

=> file reg

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001  
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STRUCTURE FILE UPDATES: 19 JUN 2001 HIGHEST RN 342573-24-4  
DICTIONARY FILE UPDATES: 19 JUN 2001 HIGHEST RN 342573-24-4

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

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=> d his

(FILE 'HOME' ENTERED AT 12:19:56 ON 20 JUN 2001)

FILE 'LREGISTRY' ENTERED AT 12:21:16 ON 20 JUN 2001

L1 STR  
L2 STR L1  
L3 STR  
L4 STR  
L5 STR L3

FILE 'REGISTRY' ENTERED AT 13:28:53 ON 20 JUN 2001

L6 0 S L2 OR L5 OR L4

FILE 'LREGISTRY' ENTERED AT 13:29:11 ON 20 JUN 2001

L7 STR

FILE 'REGISTRY' ENTERED AT 13:39:29 ON 20 JUN 2001

L8 0 S L7

FILE 'LREGISTRY' ENTERED AT 13:39:56 ON 20 JUN 2001

L9 STR L7

FILE 'REGISTRY' ENTERED AT 13:40:58 ON 20 JUN 2001

L10 18 S L9  
L11 283 S L9 FUL  
SAV L11 PAD859/A  
L12 0 S (L2 OR L5 OR L4) SSS SAM SUB=L11  
L13 2 S (L2 OR L5 OR L4) SSS FUL SUB=L11  
SAV L13 PAD859A/A  
L14 0 S L7 SSS SAM SUB=L11  
L15 5 S L7 SSS FUL SUB=L11  
SAV L15 PAD859B/A

L16 5 S L15 NOT L13

FILE 'HCA' ENTERED AT 13:48:44 ON 20 JUN 2001

L17 2 S L13  
 L18 8 S L15  
 L19 132 S L11  
 L20 75174 S (CVD OR (CHEMICAL? OR CHEM) (2A) (VAPOR? OR VAPOUR?) (2A) D  
 L21 19 S L19 AND L20  
 L22 8 S L18 NOT L17  
 L23 19 S L21 NOT (L17 OR L22)

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001

=> d 111 que stat

L9 STR

	24	27	25		
	G2	F	C		
	{	{	{		
Ta <sup>~</sup> G1	NH <sup>~</sup> G2	N <sup>~</sup> G2	@14 Ak <sup>~</sup> F	@17 Si <sup>~</sup> C	Ak @20
2 3	@5 6	@9 10	{ 15	{ 18	
			F	C	
			28	26	

VAR G1=NH2/5/9

VAR G2=20/PH/14/17

NODE ATTRIBUTES:

NSPEC IS RC AT 2  
 NSPEC IS RC AT 18  
 NSPEC IS RC AT 25  
 NSPEC IS RC AT 26  
 CONNECT IS E1 RC AT 20  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS SAT AT 20  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X4 C AT 20

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 10689 ITERATIONS

SEARCH TIME: 00.00.01

283 ANSWERS

=> d 113 que stat

L2 STR

Ta<sup>~</sup>G1  
1 2

41	42	43	44	45	46
Me	Et	n-Pr	i-Pr	n-Bu	i-Bu
N <sup>~</sup> G2	N <sup>~</sup> G3	N <sup>~</sup> G4	N <sup>~</sup> G5	N <sup>~</sup> G6	N <sup>~</sup> G7
@3	4 @5	6 @7	8 @9	10 @11	12 @13
					14

VAR G1=3/5/7/9/11/13  
 VAR G2=ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU  
 VAR G3=ME/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU  
 VAR G4=ME/ET/I-PR/N-BU/I-BU/S-BU/T-BU  
 VAR G5=ME/ET/N-PR/N-BU/I-BU/S-BU/T-BU  
 VAR G6=ME/ET/N-PR/I-PR/I-BU/S-BU/T-BU  
 VAR G7=ME/ET/N-PR/I-PR/N-BU/S-BU/T-BU

NODE ATTRIBUTES:

CONNECT IS E5 C AT 1  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L4 STR

22	25	
C	F	Ak @20
21		
C <sup>~</sup> Si <sup>~</sup> C	@18	Ak <sup>~</sup> F
24     23		19
Ta <sup>~</sup> N <sup>~</sup> G1	F	
27 3 4	26	

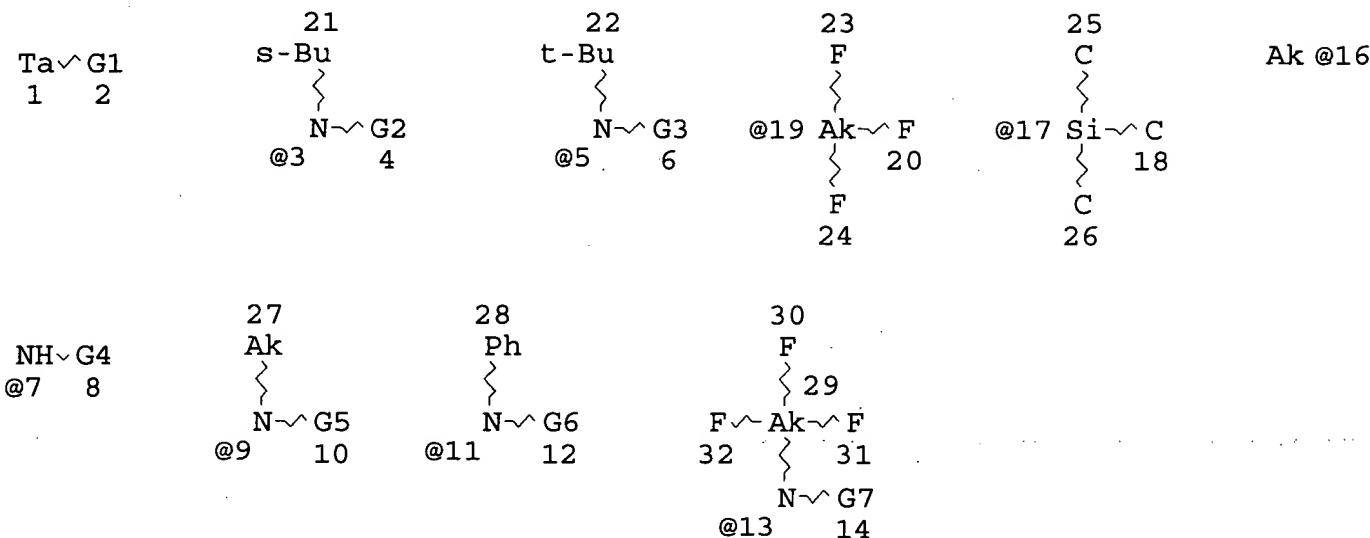
VAR G1=20/PH/18  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 22  
 NSPEC IS RC AT 23  
 NSPEC IS RC AT 24  
 CONNECT IS E1 RC AT 20  
 CONNECT IS E5 C AT 27  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS SAT AT 20  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X4 C AT 20

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 12

## STEREO ATTRIBUTES: NONE

L5 STR



VAR G1=3/5/7/9/11/13

VAR G2=ME/ET/N-PR/I-PR/N-BU/I-BU/T-BU

VAR G3=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU

VAR G4=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/PH/19/17

VAR G5=PH/19/17

VAR G6=16/19/17

VAR G7=16/PH/17

## NODE ATTRIBUTES:

NSPEC IS RC AT 18

NSPEC IS RC AT 25

NSPEC IS RC AT 26

CONNECT IS E5 C AT 1

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 27

DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 16

GGCAT IS SAT AT 27

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X4 C AT 16

ECOUNT IS M1-X4 C AT 27

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 31

## STEREO ATTRIBUTES: NONE

L9 STR

		24	27	25	
		G2	F	C	
		{	{	{	
Ta <sup>^</sup> G1	NH <sup>^</sup> G2	N <sup>~^</sup> G2	@14 Ak <sup>~^</sup> F	@17 Si <sup>~^</sup> C	Ak @20
2 3	@5 6	@9 10	{ 15	{ 18	
			F	C	
			28	26	

VAR G1=NH2/5/9  
 VAR G2=20/PH/14/17

## NODE ATTRIBUTES:

NSPEC IS RC AT 2  
 NSPEC IS RC AT 18  
 NSPEC IS RC AT 25  
 NSPEC IS RC AT 26  
 CONNECT IS E1 RC AT 20  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS SAT AT 20  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X4 C AT 20

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

## STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9  
 L13 2 SEA FILE=REGISTRY SUB=L11 SSS FUL (L2 OR L5 OR L4)

100.0% PROCESSED 283 ITERATIONS 2 ANSWERS  
 SEARCH TIME: 00.00.09

=> d l15 que stat

L7 STR

		21	24	27	25	
		G1 23	G2	F	C	
		{ G1	{	{	{	
G1 <sup>^</sup> Ta <sup>^</sup> G1	NH <sup>^</sup> G2	N <sup>~^</sup> G2	@14 Ak <sup>~^</sup> F	@17 Si <sup>~^</sup> C	Ak @20	
1 { 3	@5 6	@9 10	{ 15	{ 18		
G1			F	C		
22			28	26		

VAR G1=NH2/5/9  
 VAR G2=20/PH/14/17

## NODE ATTRIBUTES:

NSPEC IS RC AT 18  
 NSPEC IS RC AT 25  
 NSPEC IS RC AT 26  
 CONNECT IS E1 RC AT 20  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS SAT AT 20  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X4 C AT 20

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 20

## STEREO ATTRIBUTES: NONE

L9 STR

	24		27		25	
	G2		F		C	
Ta <sup>1</sup> ^ G1	NH <sup>2</sup> ^ G2	N <sup>3</sup> ^ G2	@14 Ak <sup>4</sup> ^ F	@17 Si <sup>5</sup> ^ C	Ak <sup>6</sup> @20	
2 3	@5 6	@9 10	15	18		
			F	C		
			28	26		

VAR G1=NH2/5/9

VAR G2=20/PH/14/17

## NODE ATTRIBUTES:

NSPEC IS RC AT 2  
 NSPEC IS RC AT 18  
 NSPEC IS RC AT 25  
 NSPEC IS RC AT 26  
 CONNECT IS E1 RC AT 20  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS SAT AT 20  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1-X4 C AT 20

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

## STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9  
 L15 5 SEA FILE=REGISTRY SUB=L11 SSS FUL L7

100.0% PROCESSED 283 ITERATIONS ( 5 INCOMPLETE) 5 ANSWERS  
 SEARCH TIME: 00.00.02

=> file hca

FILE 'HCA' ENTERED AT 14:13:02 ON 20 JUN 2001  
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FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26  
FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

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=> d l17 1-2 ibib abs hitstr hitind

L17 ANSWER 1 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 118:102151 HCA

TITLE: Methane vs benzene activation via transient tantalum amido-imido complex

tert-Bu3SiNHTa(:NSiBu3-tert)2: structure of (py)2MeTa(:NSiBu3-tert)2

AUTHOR(S): Schaller, Christopher P.; Wolczanski, Peter T.  
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853,  
USA

SOURCE: Inorg. Chem. (1993), 32(2), 131-44  
CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

spurk

LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 118:102151  
 AB Addn. of  $\text{Me}_3\text{TaCl}_2$  to 2.0 equiv of  $\text{LiNHSiR}_3$  ( $\text{R} = \text{CMe}_3$  throughout this abstr.) in hexanes resulted in  $\text{CH}_4$  and  $(\text{R}_3\text{SiNH})\text{Me}_2\text{Ta}:\text{NSiR}_3$  (1, 63%). Thermolysis of 1 in benzene resulted in disproportionation, but in pyridine and THF,  $\text{L}_2\text{MeTa}(:\text{NSiR}_3)_2$  ( $\text{L} = \text{py}$ , 2(py)2, 68%; THF, 2(THF)2, 13%) and  $\text{MeH}$  were produced. The bis adduct 2(py)2 is considered to form via 1,2-MeH-elimination from  $(\text{R}_3\text{SiNH})\text{Me}_2(\text{py})\text{Ta}:\text{NSiR}_3$  (1-py), which is obtained from 1 and pyridine at 25.degree..  $^1\text{H}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of 2(py)2 manifested equiv. pyridines, but an x-ray structure detn. revealed a trigonal bipyramidal, pseudo-Cs stereoisomer with an axial Me group and equatorial imides that reflects the steric requirements of the bulky  $\text{R}_3\text{SiN}$  units. Rather long  $\text{Ta}:\text{N}$  bond distances (1.810 (13) and 1.819 (13) .ANG.) support electronic arguments suggesting the imides donate a max. of 6 electrons to the metal center. Addn. of  $\text{TaCl}_5$  to 4.0 equiv of  $\text{LiNHSiR}_3$  in  $\text{Et}_2\text{O}$  at -78.degree. afforded  $(\text{R}_3\text{SiNH})_2\text{ClTa}:\text{NSiR}_3$  (3-Cl) and  $\text{R}_3\text{SiNH}_2$ . Alkylation of 3-Cl with  $\text{AlMe}_3$  (hexanes),  $\text{PhLi}$  ( $\text{Et}_2\text{O}$ /hexanes),  $\text{PhCH}_2\text{K}$  (toluene), and  $\text{RCH}_2\text{Li}$  ( $\text{Et}_2\text{O}$ ) provided  $(\text{R}_3\text{SiNH})_2\text{RTa}:\text{NSiR}_3$  ( $\text{R} = \text{Me}$ , 3-Me, 78%; Ph, 3-Ph, 64%;  $\text{CH}_2\text{Ph}$ , 3- $\text{CH}_2\text{Ph}$ , 51%;  $\text{CH}_2\text{R}$ , 3- $\text{CH}_2\text{R}$ , 39%). Addn. of  $\text{R}_3\text{SiNH}_2$  or  $\text{R}_3\text{SiOH}$  to 1 yielded 3-Me or  $(\text{R}_3\text{SiNH})(\text{R}_3\text{SiO})\text{MeTa}:\text{NSiR}_3$  (5-Me, 52%) and  $\text{CH}_4$ . Thermolysis of 3-R effected 1,2-RH-elimination to form transient  $(\text{R}_3\text{SiNH})\text{Ta}(:\text{NSiR}_3)_2$  (4), a species capable of adding C-H bonds across one imido linkage. Moderate rates of elimination from 3-R could be obtained only at 182.8 (4).degree.. Ground-state information was obtained via the approach to equil. of 3-Ph and  $\text{CH}_4$ , but observation of a p-ditantalum Ph deriv.,  
 $[(\text{R}_3\text{SiNH})_2\text{Ta}:\text{NSiR}_3]_2(\mu\ldots\eta\ldots\eta.1,\eta.1-1,4-\text{C}_6\text{H}_4) ((3)2\text{C}_6\text{H}_4)$  complicated the measurement. Simulation of the approach to equil. yielded rate consts. consistent with the previously measured 1,2-RH-elimination rates and showed that 3-Me, 3-Ph, and (3)2C6H4 possess relatively similar ground-state free energies. Equilibration of 3-CH<sub>2</sub>Ph to aryl complexes  $(\text{R}_3\text{SiNH})_2(\text{C}_6\text{H}_4\text{Me})\text{Ta}:\text{NSiR}_3$  ( $3-\text{C}_6\text{H}_4\text{Me}$ ) in toluene at 182.8 (4).degree. gave similar results. The data portray differing 1,2-RH-elimination rates that result from significant transition state energy differences, ruling out a late transition state despite a rough correlation of rate with the C-H bond strength of the eliminated alkane/arene. The implications of these measurements, including the possibility of d0 alkane or arene complexes as intermediates and differences in tantalum-carbon bond strengths, are discussed in detail.

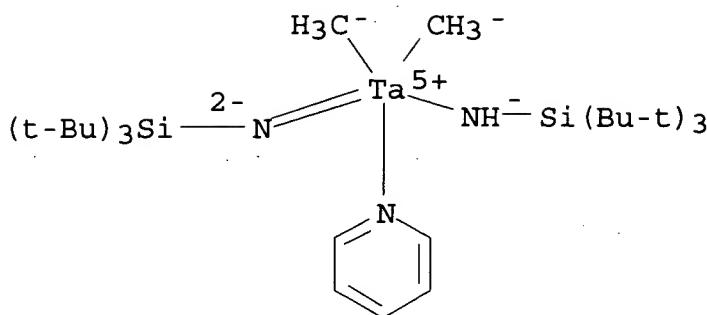
IT 146128-74-7P

(prepn. of)

RN 146128-74-7 HCA

CN Tantalum, dimethyl(pyridine)[1,1,1-tris(1,1-dimethylethyl)silanaminato][1,1,1-tris(1,1-dimethylethyl)silanaminato(2-)]- (9CI) (CA)

A INDEX NAME)  
Center group has no sign  
no van der waals  
only 3 (NRR')  
groups  
at 5



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 75

IT 145674-28-8P 145674-29-9P 145702-63-2P 146128-74-7P

146128-76-9P

(prepn. of)

L17 ANSWER 2 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 108:86837 HCA

TITLE:

Synthesis and structure of niobium(V) and tantalum(V) organoimido compounds containing 2,6-diphenylphenoxy ligation

AUTHOR(S):

Chesnut, Robert W.; Fanwick, Phillip E.; Rothwell, Ian P.

CORPORATE SOURCE:

Dep. Chem., Purdue Univ., West Lafayette, IN, 47905, USA

SOURCE:

Inorg. Chem. (1988), 27(4), 752-4

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE:

Journal

LANGUAGE:

English

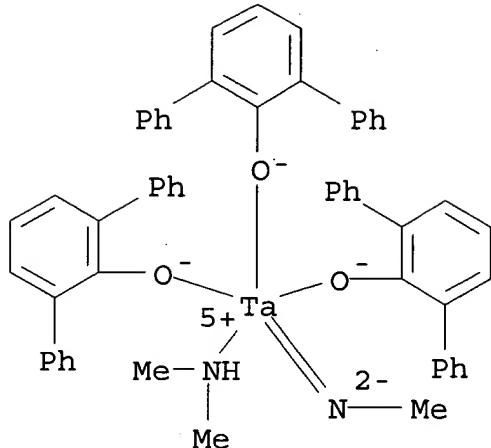
AB The addn. of 3 equiv of 2,6-diphenylphenol (HOAr-2,6Ph<sub>2</sub>) to a toluene soln. of M(NMe<sub>2</sub>)<sub>5</sub> (M = Nb, Ta) gave, on warming, M(OAr-2,6Ph<sub>2</sub>)<sub>3</sub>(NMe)(NHMe<sub>2</sub>) (I). A single crystal diffraction study of I (M = Nb) confirmed the stoichiometry and showed a geometry about the metal center best described as trigonal bipyramidal with an essentially linear Nb:NMe bond. As expected the Nb:NMe bond of 1.720(5) .ANG. is dramatically shorter than that to the amine ligand, 2.326(6) .ANG.. I (M = Nb) is orthorhombic with a = 10.808(2), b 19.499(4), c = 21.801(3) .ANG., Z = 4, d.(calcd.) = 1.305 g cm<sup>-3</sup> in space group P212121.

IT 112347-60-1P

(prepn. of)

RN 112347-60-1 HCA

CN Tantalum, [methanaminato(2-)] (N-methylmethanamine)tris([1,1':3',1'''-terphenyl]-2'-olato)-, (TB-5-12)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 75  
 IT 112347-60-1P  
 (prepn. of)

=> d 122 1-8 cbib abs hitstr hitind

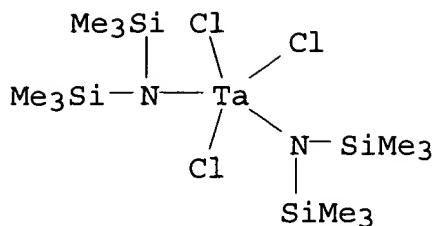
L22 ANSWER 1 OF 8 HCA COPYRIGHT 2001 ACS  
 125:184166 Synthesis and Structural Characterization of Tantalum(IV) Amido Compounds. Suh, Seigi; Hoffman, David M. (Department of Chemistry, University of Houston, Houston, TX, 77204, USA). Inorg. Chem., 35(17), 5015-5018 (English) 1996. CODEN: INOCAJ. ISSN: 0020-1669.

AB Ta(IV) amido complexes were synthesized from Ta(V) precursors.  $Ta(N(SiMe_3)_2)_2Cl_3$  reacts with Na/Hg to give  $Ta(N(SiMe_3)_2)_2Cl_2$ , and  $Ta(NEt_2)_2Cl_3$  reacts with LiNPh<sub>2</sub> and Na/Hg to yield  $Ta(NPh_2)_2(NEt_2)_2$ .  $Ta(N(SiMe_3)_2)_2Ph_2$  was prep'd. by reacting  $Ta(N(SiMe_3)_2)_2Cl_2$  with LiPh. Attempts to prep. other organometallic derivs. failed to yield clean products. X-ray crystallog. studies show that  $Ta(N(SiMe_3)_2)_2Cl_2$ ,  $Ta(N(SiMe_3)_2)_2Ph_2$ , and  $Ta(NPh_2)_2(NEt_2)_2$  have distorted tetrahedral geometries.

IT 71616-54-1, Trichlorobis(bis(trimethylsilyl)amido)tantalum  
 (for prepn. of tantalum 4 amido complexes)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 29, 75

IT 591-51-5, Phenyllithium 5856-89-3, Lithium diphenylamide  
**71616-54-1**, Trichlorobis(trimethylsilyl)amido tantalum  
 99449-55-5

(for prepn. of tantalum 4 amido complexes)

L22 ANSWER 2 OF 8 HCA COPYRIGHT 2001 ACS

119:61653 Syntheses and crystal structure of tantalum(IV) amido and imido halide complexes. Hoffman, David M.; Suh, Seigi (Dep. Chem., Univ. Houston, Houston, TX, 77204, USA). J. Chem. Soc., Chem. Commun. (8), 714-15 (English) 1993. CODEN: JCCCAT. ISSN: 0022-4936.

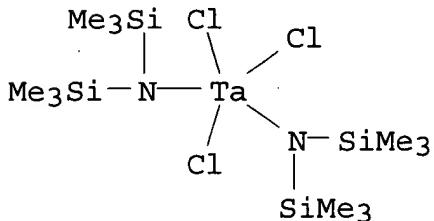
AB The syntheses and crystal structures of monomeric Ta(IV) amido halide and dimeric Ta(IV) imido halide complexes are reported. Ta[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>Cl<sub>3</sub> was reduced by Na/Hg to give Ta[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>Cl<sub>2</sub> (I). Ta(NSiMe<sub>3</sub>)[N(SiMe<sub>3</sub>)<sub>2</sub>]Cl<sub>2</sub>(THF) was similarly reduced to give {Ta(.mu.-NSiMe<sub>3</sub>)[N(SiMe<sub>3</sub>)<sub>2</sub>]Cl}<sub>2</sub> (II). I and II were characterized by elemental anal., NMR and IR spectrometries, and x-ray crystallog. I has a severely distorted tetrahedral geometry. II has an edge-shared tetrahedral structure and a Ta-Ta distance of 2.621(1) .ANG..

IT **71616-54-1**

(redn. of, by sodium amalgam)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



3(Cl)

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT **71616-54-1** 134588-18-4  
 (redn. of, by sodium amalgam)

L22 ANSWER 3 OF 8 HCA COPYRIGHT 2001 ACS

115:20938 Organoimidotantalum(V) complexes containing halide, dialkylamide, monoalkylamide, alkoxide, aryloxide, trialkylphosphine and tetrahydrofuran ligands. Crystal structures of  $[\{Ta(\mu\text{-Cl})Cl(\text{NSiMe}_3)[N(\text{SiMe}_3)_2]\}_2]$  and  $[\{Ta(\mu\text{-OMe})(\text{OMe})(\text{NSiMe}_3)[N(\text{SiMe}_3)_2]\}_2]$ . Bradley, Donald C.; Hursthouse, Michael B.; Howes, Andrew J.; Jelfs, Alasdair N. de M.; Runnacles, John D.; Thornton-Pett, Mark (Dep. Chem., Queen Mary and Westfield Coll., London, E1 4NS, UK). J. Chem. Soc., Dalton Trans. (150th Anniv. Celebration Issue), 841-7 (English) 1991. CODEN: JCDTBI. ISSN: 0300-9246.

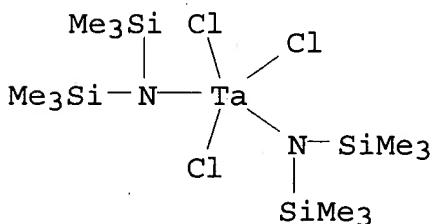
AB By means of various reactions  $[TaCl_3\{N(\text{SiMe}_3)_2\}_2]$  was converted into the  $[\{Ta(\mu\text{-X})(\text{NSiMe}_3)[N(\text{SiMe}_3)_2]\}_2]$  (I: X = Cl, I),  $[TaCl_2(\text{NSiMe}_3)\{N(\text{SiMe}_3)_2\}(\text{THF})]$ ,  $[Ta(\text{NET})(\text{NHET})\{N(\text{SiMe}_3)_2\}_2]$ , and  $[Ta(\text{NCMe}_3)(\text{NHET})\{N(\text{SiMe}_3)_2\}_2]$ . From I (X = Cl)  $[Ta(\text{NSiMe}_3)\{N(\text{SiMe}_3)_2\}(\text{NHCM}_3)_2]$ ,  $[Ta(\text{NSiMe}_3)\{N(\text{SiMe}_3)_2\}(\text{OCMe}_3)_2]$ , and  $[\{Ta(\mu\text{-OMe})(\text{OMe})(\text{NSiMe}_3)[N(\text{SiMe}_3)_2]\}_2]$  (II) were obtained and from  $[TaCl_3(\text{OC}_6\text{H}_2\text{Me}(\text{CMe}_3)_2)_2]$ ,  $[Ta(\text{NET})(\text{NHET})(\text{OC}_6\text{H}_2\text{Me}(\text{CMe}_3)_2)_2]$ ,  $[Ta(\text{NCH}_2\text{CMe}_3)(\text{NHCH}_2\text{CMe}_3)(\text{OC}_6\text{H}_2\text{Me}(\text{CMe}_3)_2)_2]$ , and  $[Ta(\text{NCMe}_3)(\text{NHCM}_3)(\text{OCH}_2\text{Me}(\text{CMe}_3)_2)_2]$  were prep'd.  $[TaCl_3(\text{NPh})(\text{PEt}_3)_2]$  and  $[TaCl_3(\text{NPh})(\text{PEt}_2\text{Ph})_2]$  were prep'd. from reaction involving  $\text{NPh}(\text{SiMe}_3)$  and  $\text{TaCl}_5$  in the presence of trialkylphosphines. All of these new compds. were characterized by NMR, IR, and mass spectra and I (X = Cl) and II were structurally characterized by single-crystal x-ray crystallog. I (X = Cl) is triclinic, space group P.hivin.1, Z = 1, R = 0.035, R1 = 0.040; II is monoclinic, space group P21/n, Z = 2, R = 0.057, R1 = 0.051...

IT 71616-54-1

(reaction of, with iodotrimethylsilane and THF and ethylamide)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 75

IT 71616-54-1

(reaction of, with iodotrimethylsilane and THF and ethylamide)

L22 ANSWER 4 OF 8 HCA COPYRIGHT 2001 ACS

101:182554 Organoimido complexes of tantalum(V). Preparation and x-ray crystal structure of bis[bis(trimethylsilyl)amido]chloro(tert-

butylimido)tantalum(V) and bis(trimethylsilyl)amido-di-.mu.-bromodibromobis(trimethylsilylimido)ditantalum(V). Bradley, Donald C.; Hursthouse, Michael B.; Malik, K. M. Abdul; Nielson, Alistair J.; Chota Vuru, George B. (Dep. Chem., Queen Mary Coll., London, E1 4NS, UK). J. Chem. Soc., Dalton Trans. (6), 1069-72 (English) 1984. CODEN: JCDTBI. ISSN: 0300-9246.

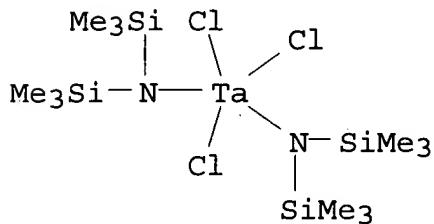
AB Reaction of  $TaCl_3[N(SiMe_3)_2]_2$  (I) with  $LiNHMe_3$  in pentane for 15 h gave 71%  $TaCl[N(CMe_3)_2]_2$  (II). I with  $Me_3SiBr$  in refluxing PhMe for 6 h gave 25%  $[TaBr_2(NSiMe_3)[N(SiMe_3)_2]]_2$  (III), a centrosym. 5-coordinated dimer. II is monoclinic, space group  $P2_1/n$ , with a 12.343(2), b 19.089(3), c 12.135(3) .ANG., .beta. 94.98(3).degree., Z = 4, d.(calcd.) = 1.42 g cm<sup>-3</sup>, R = 0.041. III is triclinic, space group P.hivin.1, with a 9.254(4), b 9.340(4), c 12.287(5), .alpha. 87.57(4), .beta. 84.04(4), .gamma. 102.30(4).degree., Z = 1, d.(calcd.) = 1.905 g cm<sup>-3</sup>, R = 0.053. Treatment of III with pyridine or  $PM_3$  cleaved the unsym. Br bridge to give  $TaBr_2(NSiMe_3)[N(SiMe_3)_2]L$  (L = py,  $PM_3$ ). Reaction of I with  $NaS_2CNMe_2$  gave  $Ta(NSiMe_3)(S_2CNMe_2)_3(CH_2Cl_2)$ , which may involve a 7-coordinated Ta imido complex.

IT 71616-54-1

(substitution reactions of, imido complexes by)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT 71616-54-1

(substitution reactions of, imido complexes by)

L22 ANSWER 5 OF 8 HCA COPYRIGHT 2001 ACS

93:8260 The preparation, characterization and crystal and molecular structure of bis(bis(trimethylsilyl)amido)trichlorotantalum(V). Bradley, Donald C.; Hursthouse, Michael B.; Malik, K. M. Abdul; Vuru, George B. C. (Dep. Chem., Queen Mary Coll., London, E1 4NS, Engl.). Inorg. Chim. Acta, 44(1), L5-L6 (English) 1980. CODEN: ICHAA3. ISSN: 0020-1693.

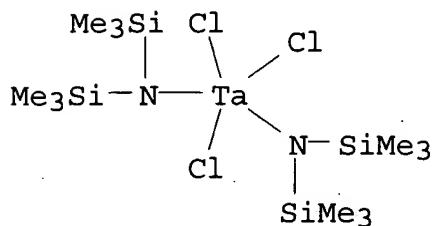
AB In the reaction with  $LiN(SiMe_3)_2$ ,  $TaCl_5$  underwent only disubstitution to give  $TaCl_3[N(SiMe_3)_2]_2$  (I), irresp. of the  $LiN(SiMe_3)_2$ - $TaCl_5$  mol ratio (1-5) in pentane. Structure detns. of I indicated that it had a distorted trigonal bipyramidal structure in which the bulky  $N(SiMe_3)_2$  groups occupied equatorial sites.

IT **71616-54-1P**

(prepn. and structure of)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT **71616-54-1P**

(prepn. and structure of)

L22 ANSWER 6 OF 8 HCA COPYRIGHT 2001 ACS

93:8233 A convenient preparation of metal pseudohalide compounds.

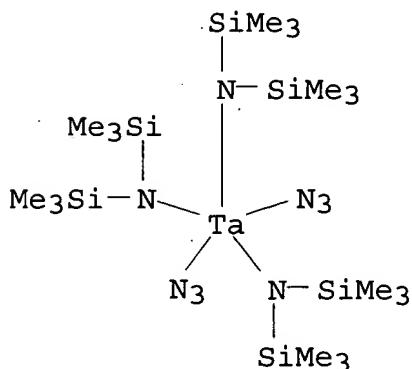
Andersen, Richard A. (Chem. Dep., Univ. California, Berkeley, CA, 94720, USA). Inorg. Nucl. Chem. Lett., 16(1), 31-2 (English) 1980.  
CODEN: INUCAF. ISSN: 0020-1650.

AB A reaction of [(Me<sub>3</sub>Si)<sub>2</sub>N]<sub>3</sub>HfCl with Me<sub>3</sub>SiX gave [(Me<sub>3</sub>Si)<sub>2</sub>N]<sub>3</sub>HfX (X = Br, I, N<sub>3</sub>, CN), quant. [(Me<sub>3</sub>Si)<sub>2</sub>N]<sub>2</sub>Ta(N<sub>3</sub>)<sub>3</sub> was similarly prepd.IT **73830-77-0P**

(prepn. of)

RN 73830-77-0 HCA

CN Tantalum, diazidotris[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]- (9CI) (CA INDEX NAME)

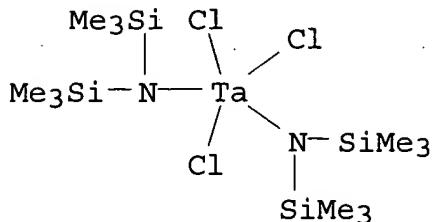
IT **71616-54-1**

(reaction of, with trimethylsilyl azide)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-

(trimethylsilyl)silanaminato] -, (SP-5-11) - (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 73830-74-7P 73830-75-8P 73830-76-9P **73830-77-0P**  
73841-10-8P

(prepn. of)

IT **71616-54-1**

(reaction of, with trimethylsilyl azide)

L22 ANSWER 7 OF 8 HCA COPYRIGHT 2001 ACS

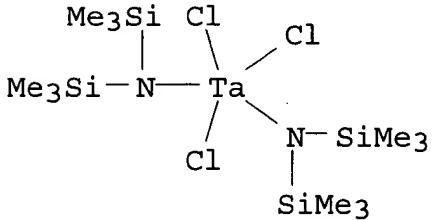
91:211518 Trimethylbis[bis(trimethylsilyl)amido]tantalum(V) and  
[(trimethylsilyl)methyl][trimethylsilylmethylidene]bis[trimethylsilyl]amido]tantalum(V). Andersen, Richard A. (Dep. Chem., Univ. California, Berkeley, CA, 94720, USA). Inorg. Chem., 18(12), 3622-3 (English) 1979. CODEN: INOCAJ. ISSN: 0020-1669.

AB Bis(hexamethyldisilylamido)trichlorotantalum, from Na hexamethyldisilylamide and TaCl<sub>5</sub>, yields Me<sub>3</sub>Ta[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub> upon reaction with MeLi. The structure of this five-coordinate species is most reasonably described as a square pyramid with hexamethyldisilylamido ligands trans to each other and cis to the 3 Me-Ta groups. The carbene complex, (Me<sub>3</sub>SiCH<sub>2</sub>)(Me<sub>3</sub>SiCH)Ta[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>, is formed from the trichloride and Me<sub>3</sub>SiCH<sub>2</sub>Li.

IT **71616-54-1P 71616-55-2P**  
(prepn. of)

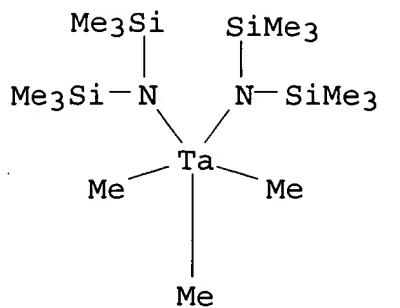
RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato] -, (SP-5-11) - (9CI) (CA INDEX NAME)



RN 71616-55-2 HCA

CN Tantalum, trimethylbis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato] -, (SP-5-21) - (9CI) (CA INDEX NAME)



$2(N^+)$   
 $3(ne)$

L22 ANSWER 8 OF 8 HCA COPYRIGHT 2001 ACS

81:32725 Complexes of tantalum and antimony pentafluorides with dimethyl ether and trimethylamine. Brownstein, S.; Farrall, Marjorie J. (Div. Chem., Natl. Res. Counc. Canada, Ottawa, Ont., Can.). Can. J. Chem., 52(10), 1958-65 (English) 1974. CODEN: CJCHAG.

AB TaF<sub>5</sub> forms 1:1 and 1:2 complexes with Me<sub>2</sub>O and Me<sub>3</sub>N. SbF<sub>5</sub> forms 2:1 and 1:1 complexes with Me<sub>2</sub>O and Me<sub>3</sub>N. The rates of exchange of terminal and equatorial fluorines in the 1:1 TaF<sub>5</sub>-Me<sub>2</sub>O adduct are measured.

IT 53129-67-2

(exchange of fluorine in, NMR in relation to)

RN 53129-67-2 HCA

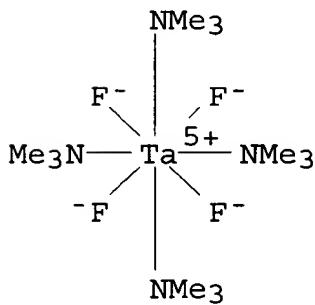
CN Tantalum(1+), tetrakis(N,N-dimethylmethanamine)tetrafluoro-  
(OC-6-11)-hexafluorotantalate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 53129-66-1

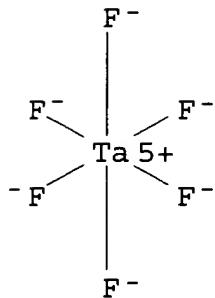
CMF C12 H36 F4 N4 Ta

CCI CCS



CM 2

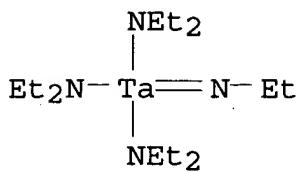
CRN 16918-70-0  
 CMF F6 Ta  
 CCI CCS  
 CDES 7:OC-6-11



CC 78-9 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 67  
 IT 12122-12-2 53129-63-8 53129-65-0 **53129-67-2**  
 53129-68-3 53129-69-4 53129-70-7  
 (exchange of fluorine in, NMR in relation to)

=> d 123 1-19 cbib abs hitstr hitind

L23 ANSWER 1 OF 19 HCA COPYRIGHT 2001 ACS  
 134:374292 Tantalum-carbon thin films for low-resistivity barrier layers  
 and their manufacture by **MOCVD**. Nakamura, Satoshi;  
 Komatsu, Takashi; Higuchi, Yasushi; Nagano, Kenzo; Taguma, Yasuhiro  
 (ULVC Japan, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2001131746 A2  
 20010515, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP  
 1999-318244 19991109.  
 AB The process comprises deposition of C-rich layers on substrates by  
**MOCVD** and plasma exposure of the layers while applying bias  
 potential on the substrates to give Ta-C layers with resistivity  
 350-2000 .mu..OMEGA.cm. The **MOCVD** sources may be  
 alkylaminotantalum compds.  
 IT **67313-80-8**  
 (source; manuf. of Ta-C thin films for low-resistivity barrier  
 layers by **MOCVD** and followed plasma exposure)  
 RN 67313-80-8 HCA  
 CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)  
 (CA INDEX NAME)



IC ICM C23C016-32  
ICS H01L021-285; H01L021-3205

CC 75-1 (Crystallography and Liquid Crystals)  
Section cross-reference(s): 76

ST tantalum carbon barrier layer low resistivity; MOCVD  
plasma annealing tantalum carbon layer; alkylaminotantalum  
MOCVD tantalum carbon barrier layer

IT Electric conductors  
(barrier layers; manuf. of Ta-C thin films for low-resistivity  
barrier layers by **MOCVD** and followed plasma exposure)

IT Bias potential  
Plasma  
(manuf. of Ta-C thin films for low-resistivity barrier layers by  
**MOCVD** and followed plasma exposure)

IT Vapor deposition process  
(metalorg.; manuf. of Ta-C thin films for low-resistivity barrier  
layers by **MOCVD** and followed plasma exposure)

IT Annealing  
(plasma; manuf. of Ta-C thin films for low-resistivity barrier  
layers by **MOCVD** and followed plasma exposure)

IT 164992-28-3P  
(manuf. of Ta-C thin films for low-resistivity barrier layers by  
**MOCVD** and followed plasma exposure)

IT 7439-90-9, Krypton, uses 7440-37-1, Argon, uses 7440-63-3,  
Xenon, uses 7727-37-9, Nitrogen, uses  
(plasma contg.; manuf. of Ta-C thin films for low-resistivity  
barrier layers by **MOCVD** and followed plasma exposure)

IT **67313-80-8**  
(source; manuf. of Ta-C thin films for low-resistivity barrier  
layers by **MOCVD** and followed plasma exposure)

L23 ANSWER 2 OF 19 HCA COPYRIGHT 2001 ACS

134:319599 Method for fabricating gate oxide layer for a semiconductor device. Huang, Kuo-Tai; Huang, Michael W. C.; Yew, Tri-Rung (United Microelectronics Corp., Taiwan). U.S. US 6221712 B1 20010424, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 1999-385805 19990830.

AB A method is provided for fabricating a gate structure. The method involves providing a substrate, followed by forming a nitride region on a surface of the substrate. With a Ta-based org. compd. and a Ti-based org. compd. serving as precursors, an metalorg. CVD (**MOCVD**) is performed, so that a Ta<sub>2-x</sub>Ti<sub>x</sub>O<sub>5</sub> dielec. layer is formed on the substrate. A barrier layer, a conducting layer, and an anti-reflection (AR) layer are then formed in sequence on the Ta<sub>2-x</sub>Ti<sub>x</sub>O<sub>5</sub> dielec. layer. Subsequently, the AR layer, the

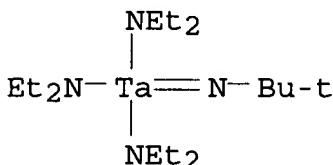
conducting layer, the barrier layer, and the  $Ta_{2-x}Ti_xO_5$  dielec. layer are defined to form a gate structure on the substrate of the nitride region. The Ta-based org. compd. in this case may include a Ta-alkoxide compd., whereas the Ti-based org. compd. may include a Ti-alkoxide compd. or a Ti-amide compd.

\* IT **169896-41-7**

(vapor deposition precursor; method for fabricating gate oxide layer for a semiconductor device)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM B32B019-00

NCL 438240000

CC 76-3 (Electric Phenomena)

IT 546-68-9, Titanium tetra-isopropoxide 3087-39-6, Titanium tetrakis(t-butoxide) 3275-24-9, Titanium tetrakis(dimethylamide) 4419-47-0, Titanium tetrakis(diethylamide) 6074-84-6, Tantalum ethoxide 52406-69-6 52406-81-2 **169896-41-7**  
172901-22-3 177580-52-8 177580-53-9 238757-13-6

(vapor deposition precursor; method for fabricating gate oxide layer for a semiconductor device)

L23 ANSWER 3 OF 19 HCA COPYRIGHT 2001 ACS

134:260170 Formation of dielectric layer of capacitor. Fuang, Guo Tai; You, Cui Rong (Lien Hua Electronics Co., Ltd., Taiwan). Jpn. Kokai Tokkyo Koho JP 2001085423 A2 20010330, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-256379 19990909.

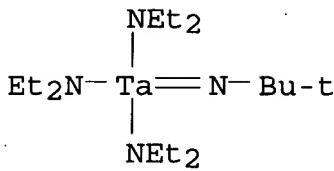
AB The title method involves prep. an org. compd. contg. Ta and an org. compd. contg. Ti, and carrying out MOCVD using the org. compds. as precursors. A dielec. layer of tantalum titanium oxide having a high dielec. const. is formed. A method is also described, for forming a capacitor of a DRAM using the above method.

IT **169896-41-7**

(MOCVD of tantalum titanium oxide dielec. layer of capacitor)

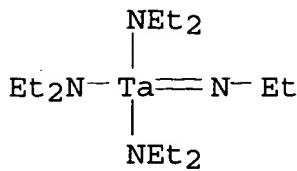
RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM H01L021-316  
 ICS C23C016-40; H01L021-31; H01L027-108; H01L021-8242; H01G004-33;  
 H01G004-10  
 CC 76-10 (Electric Phenomena)  
 Section cross-reference(s): 75  
 ST MOCVD tantalum titanium oxide dielec film DRAM capacitor  
 IT Memory devices  
     (DRAM (dynamic random access); MOCVD of tantalum  
     titanium oxide dielec. layer of capacitor)  
 IT Capacitors  
 Dielectric films  
     (MOCVD of tantalum titanium oxide dielec. layer of  
     capacitor)  
 IT Vapor deposition process  
     (metalorg.; MOCVD of tantalum titanium oxide dielec.  
     layer of capacitor)  
 IT 60866-78-6, Tantalum titanium oxide  
     (MOCVD of tantalum titanium oxide dielec. layer of  
     capacitor)  
 IT 546-68-9, Titanium tetraisopropoxide 3087-39-6 3275-24-9,  
 Titanium tetrakisdimethylamide 4419-47-0, Titanium  
 tetrakisdiethylamide 6074-84-6, Tantalum pentaethoxide  
 52406-69-6 169896-41-7 172901-22-3 177580-52-8  
 177580-53-9 238757-13-6  
     (MOCVD of tantalum titanium oxide dielec. layer of  
     capacitor)

L23 ANSWER 4 OF 19 HCA COPYRIGHT 2001 ACS  
 134:108338 MOCVD of tantalum nitride (TaN<sub>x</sub>, x=0.3-1.5) film.  
 Nagano, Kenzo; Nakamura, Satoshi; Komatsu, Takashi; Higuchi,  
 Yasushi; Taguma, Yasuhiro (ULVC Japan, Ltd., Japan). Jpn. Kokai  
 Tokkyo Koho JP 2001011631 A2 20010116, 4 pp. (Japanese). CODEN:  
 JKXXAF. APPLICATION: JP 1999-183563 [19990629] — *not pursued*  
 AB The title method involves using ammonia and a metalorg. precursor  
 mixt. of a metalorg. compd. having a Ta=N double bond and a  
 metalorg. compd. free of a Ta=N double bond. The tantalum nitride  
 film is useful as a barrier film of a semiconductor device.  
 IT 67313-80-8  
     (precursors for MOCVD of tantalum nitride (TaN<sub>x</sub>,  
     x=0.3-1.5) film useful for semiconductor device barrier)  
 RN 67313-80-8 HCA  
 CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4) - (9CI)  
     (CA INDEX NAME)



IC ICM C23C016-34  
 ICS H01L021-285  
 CC 75-1 (Crystallography and Liquid Crystals)  
 Section cross-reference(s): 76  
 ST MOCVD tantalum nitride barrier semiconductor device  
 IT Vapor deposition process  
     (metalorg.; precursors for MOCVD of tantalum nitride  
     (TaN<sub>x</sub>, x=0.3-1.5) film useful for semiconductor device barrier)  
 IT Diffusion barrier  
 Semiconductor device fabrication  
 Semiconductor devices  
     (precursors for MOCVD of tantalum nitride (TaN<sub>x</sub>,  
     x=0.3-1.5) film useful for semiconductor device barrier)  
 IT 7664-41-7, Ammonia, uses 67313-80-8 98145-63-2  
     (precursors for MOCVD of tantalum nitride (TaN<sub>x</sub>,  
     x=0.3-1.5) film useful for semiconductor device barrier)  
 IT 12033-62-4, Tantalum nitride (TaN) 12033-63-5, Tantalum nitride  
     (TaN<sub>0.5</sub>) 122362-88-3, Tantalum nitride (TaN<sub>0.8</sub>) 150533-60-1,  
     Tantalum nitride (TaN<sub>0.2</sub>) 318522-19-9, Tantalum nitride  
     (TaN<sub>0.3-1.5</sub>)  
     (precursors for MOCVD of tantalum nitride (TaN<sub>x</sub>,  
     x=0.3-1.5) film useful for semiconductor device barrier)

L23 ANSWER 5 OF 19 HCA COPYRIGHT 2001 ACS

134:94293 Liquid precursor mixtures for deposition of multicomponent  
 metal containing electronic materials. Senzaki, Yoshihide; Roberts,  
 David Allen; Norman, John Anthony Thomas (Air Products and  
 Chemicals, Inc., USA). Eur. Pat. Appl. EP 1067595 A2 20010110, 8  
 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT,  
 LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN:  
 EPXXDW. APPLICATION: EP 2000-114321 20000704. PRIORITY: US  
 1999-350074 19990708.

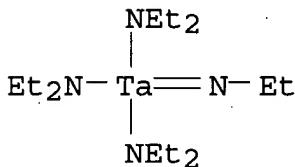
AB The process for deposition of a multiple metal or metal compd. layer  
 on a substrate of an electronic material comprises providing a  
 solventless mixt. of .gtoreq.2 metal-ligand complex precursors which  
 constitute a liq. at ambient conditions, in which the ligands are  
 the same and are selected from the group consisting of alkyls,  
 alkoxides, halides, hydrides, amides, imides, azides, nitrates,  
 cyclopentadienyls, carbonyls, and their F, O and N substituted  
 analogs. The solventless mixt. are delivered by direct liq.  
 injection to a flash vaporization zone to vaporize the solventless  
 mixt., and a resulting vapor of the solventless mixt. is contacted  
 with a substrate under deposition conditions to deposit a multiple  
 metal or metal compd. layer on the substrate. Alternatively, the

solventless mixt. is delivered to a deposition zone where a substrate is located; and the substrate under deposition conditions is contacted with the solventless mixt. to deposit a multiple metal or metal compd. layer on the substrate. The contacting process on the substrate is selected from the group consisting of **chem** **vapor deposition**, spray pyrolysis, sol-gel processing, spin coating, and at. layer epitaxy.

IT 67313-80-8

(liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)  
(CA INDEX NAME)

IC ICM H01L021-288

CC 76-3 (Electric Phenomena)

Section cross-reference(s): 75

IT **Vapor deposition process**

(chem.; liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

IT 555-75-9 1071-76-7 1624-01-7 3275-24-9 4419-47-0 5593-70-4  
6074-84-6 13801-49-5 14254-05-8 19756-04-8 19824-55-6  
19824-57-8 19824-59-0 19824-60-3 25169-05-5 62029-51-0  
**67313-80-8** 70599-04-1 220613-03-6 318277-04-2  
318277-05-3 318277-06-4 318277-07-5

(liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

L23 ANSWER 6 OF 19 HCA COPYRIGHT 2001 ACS

134:64030 Metalorganic CVD of tantalum oxide from tert-butylimidotris(diethylamido)tantalum and oxygen. Chiu, Hsin-Tien; Wang, Chun-Nan; Chuang, Shiow-Huey (Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 30050, Taiwan). Chem. Vap. Deposition, 6(5), 223-225 Published in: Adv. Mater. (Weinheim, Ger.), 12(19) (English) 2000. CODEN: CVDFX. ISSN: 0948-1907. Publisher: Wiley-VCH Verlag GmbH.

AB The results are reported of preliminary exploration of metalorg. CVD of tantalum oxide from tert-butylimidotris(diethylamido)tantalum and oxygen.

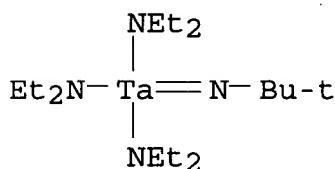
Tert-butylimidotris(diethylamido)tantalum, (TBTDET) with a higher vapor pressure than Ta(OEt)<sub>5</sub>, and other tantalum alkoxides, can be used as a precursor to grow tantalum oxide thin films by CVD for device application. Using this precursor, a Ta<sub>2</sub>O<sub>5</sub> film with a thickness of 180 nm had a leakage c.d. below 1 .times. 10<sup>-8</sup> A/cm<sup>2</sup>

for an elec. field strength of 2 MV/cm, and a breakdown voltage of 2 MV/cm. The dielec. const. was 22.

IT 169896-41-7, tert-Butylimidotris(diethylamido)tantalum  
(metalorg. CVD and elec. properties of tantalum oxide  
from tert-butylimidotris(diethylamido)tantalum and oxygen for  
device application)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-,  
(T-4)- (9CI) (CA INDEX NAME)



CC 75-1 (Crystallography and Liquid Crystals)

Section cross-reference(s): 76

ST metalorg CVD tantalum oxide butylimidotrisdiethylamidotant  
alum oxygen

IT Dielectric constant

Electric field

Leakage current

Semiconductor devices

(metalorg. CVD and elec. properties of tantalum oxide  
from tert-butylimidotris(diethylamido)tantalum and oxygen for  
device application)

IT Vapor deposition process

(metalorg.; metalorg. CVD and elec. properties of  
tantalum oxide from tert-butylimidotris(diethylamido)tantalum and  
oxygen for device application)

IT 1314-61-0, Tantalum oxide Ta2O5

(metalorg. CVD and elec. properties of tantalum oxide  
from tert-butylimidotris(diethylamido)tantalum and oxygen for  
device application)

IT 7782-44-7, Oxygen, reactions 169896-41-7,

tert-Butylimidotris(diethylamido)tantalum

(metalorg. CVD and elec. properties of tantalum oxide  
from tert-butylimidotris(diethylamido)tantalum and oxygen for  
device application)

L23 ANSWER 7 OF 19 HCA COPYRIGHT 2001 ACS

133:289409 MOCVD of high-K dielectrics and conductive metal

nitride thin films. Senzaki, Yoshihide; Hamilton, Richard F.; Reid,  
Kimberly G.; Hobbs, Christopher C.; Hegde, Rama I.; Tiner, Mike J.  
(Schumacher, Carlsbad, CA, 92009, USA). Mater. Res. Symp.  
Proc., 606 (Chemical Processing of Dielectrics, Insulators and  
Electronic Ceramics), 13-22 (English) 2000. CODEN: MRSPDH. ISSN:  
0272-9172. Publisher: Materials Research Society.

AB A known liq. mixt. of  $[(\text{CH}_3\text{CH}_2)_2\text{N}]_3\text{Ta}=\text{NCH}_2\text{CH}_3$  and

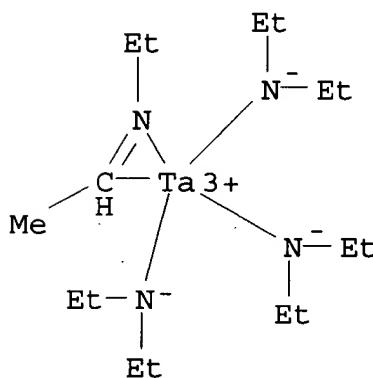
$[(CH_3CH_2)_2N]_3Ta[.eta.2-CH_3CH_2N=CH(CH_3)]$  was studied to deposit Ta<sub>2</sub>O<sub>5</sub> and TaN thin films by CVD. Films were deposited at temps. below 400.degree.C using oxygen for oxide and ammonia for nitride, resp. XRD anal. revealed that as-deposited amorphous tantalum oxide films were converted to hexagonal Ta<sub>2</sub>O<sub>5</sub> after annealing under oxygen, while tantalum nitride thin films contained cubic TaN as deposited. The low viscosity, thermal stability, and sufficient volatility of the precursor allows direct liq. injection to deliver the precursor, which results in high deposition rate and uniformity of the deposited films.

IT 67296-24-6 67313-80-8 300408-20-2

(MOCVD of high-K dielecs. and conductive metal nitride thin films)

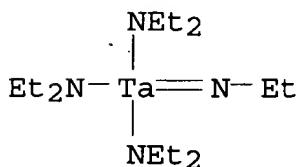
RN 67296-24-6 HCA

CN Tantalum, tris(N-ethylethanaminato)(.eta.2-N-ethylideneethanamine) - (9CI) (CA INDEX NAME)



RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4) - (9CI) (CA INDEX NAME)



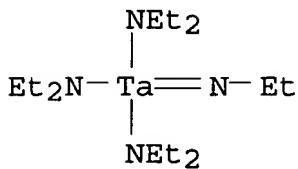
RN 300408-20-2 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4) -, mixt. with tris(N-ethylethanaminato)(.eta.2-N-ethylideneethanamine)tantalum (9CI) (CA INDEX NAME)

CM 1

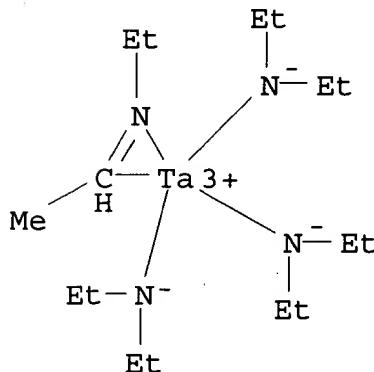
CRN 67313-80-8

CMF C14 H35 N4 Ta  
CDES 7:T-4



CM 2

CRN 67296-24-6  
CMF C16 H39 N4 Ta  
CCI CCS



CC 76-3 (Electric Phenomena)  
Section cross-reference(s): 75  
ST MOCVD tantalum oxide nitride film  
IT Annealing  
Controlled atmospheres  
Crystallization  
Dielectric constant  
Dielectric films  
Leakage current  
Semiconductor device fabrication  
(MOCVD of high-K dielecs. and conductive metal nitride  
thin films)  
IT Films  
(elec. conductive; MOCVD of high-K dielecs. and  
conductive metal nitride thin films)  
IT Electric conductors  
(films; MOCVD of high-K dielecs. and conductive metal  
nitride thin films)  
IT Vapor deposition process

(metalorg.; **MOCVD** of high-K dielecs. and conductive metal nitride thin films)

IT 1314-61-0, Tantalum pentoxide 12033-62-4, Tantalum nitride TaN  
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)

IT 7782-44-7, Oxygen, processes  
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)

IT 67296-24-6 67313-80-8 300408-20-2  
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)

IT 7664-41-7, Ammonia, reactions  
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)

L23 ANSWER 8 OF 19 HCA COPYRIGHT 2001 ACS

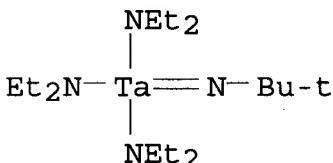
133:97909 Formation of copper thin films by **chemical vapor deposition**. Kusumoto, Toshiro; Murata, Masaaki; Ichihashi, Motoko (ULVC Japan, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2000195863 A2 20000714, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-370603 19981225.

AB The processes involves depositing TiN or TaN thin films on substrates with barrier metal films by **CVD**, followed with depositing Cu thin films by **CVD**. The raw materials for Cu thin film deposition may be Cu(I) (HFAC) VTMS or Cu(II) (HFAC) 2. The raw materials for TiN film may be Ti(NMe<sub>2</sub>)<sub>4</sub>, Ti(NEt<sub>2</sub>)<sub>4</sub>, and/or Ti(i-PrNMe)<sub>4</sub> and the raw materials for TaN may be Ta(NMe<sub>2</sub>)<sub>5</sub> and/or Ta:N(tert-butyl)(NMe<sub>2</sub>)<sub>3</sub>. The **CVD**-Cu film have excellent adhesion and smoothness.

IT 169896-41-7  
(formation of copper thin films on substrates with barrier metal films by **CVD**)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethyllethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM H01L021-3205  
ICS C23C016-18; C23C016-34; H01L021-285

CC 76-3 (Electric Phenomena)

ST copper thin film formation CVD underlayer; titanium nitride underlayer copper thin film CVD; tantalum nitride underlayer copper thin film CVD

IT 7440-50-8P, Copper, preparation  
(formation of copper thin films on substrates with barrier metal

films by CVD)

IT 3275-24-9, Tetrakis(dimethylamino)titanium 4419-47-0,  
 Tetrakis(diethylamino)titanium 14781-45-4 19824-59-0,  
 Pentakis(dimethylamino)tantalum 139566-53-3, Copper(I)  
 hexafluoroacetylacetone trimethylvinylsilane **169896-41-7**  
 282107-41-9  
 (formation of copper thin films on substrates with barrier metal  
 films by CVD)

IT 12033-62-4, Tantalum nitride 25583-20-4, Titanium nitride  
 (thin films, formation of, by CVD; formation of copper  
 thin films on substrates with barrier metal films by CVD  
 )

L23 ANSWER 9 OF 19 HCA COPYRIGHT 2001 ACS

132:238802 **Chemical vapor deposition**

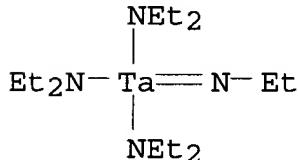
process and device manufactured by the method. Machida, Hideaki;  
 Higuchi, Noboru; Kokubu, Hiroshi; Funakubo, Hiroshi (Tori Chemical  
 Kenkyusho K. K., Japan). Jpn. Kokai Tokkyo Koho JP 2000087240 A2  
 20000328, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP  
 1998-256867 19980910.

AB The method involves using an org. metal compd. having free groups  
 and performing vapor transport using a carrier gas contg. a compd.  
 having the groups or a compd. having the groups as a carrier gas. A  
 Ca-, Sr-, Ba-, Pb-, Ta-, Cu-, Ti-, Zr-, and Al-based film are  
 manufd. by the method. Stable vapor transport is performed in the  
 CVD process with decompn. prevention of the compd.

IT **67313-80-8 169896-41-7**  
 (film formation by CVD for dielec. devices)

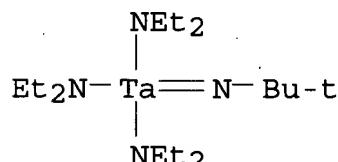
RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)  
 (CA INDEX NAME)



RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-,  
 (T-4)- (9CI) (CA INDEX NAME)



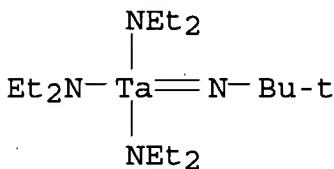
IC ICM C23C016-18  
 ICS C01G029-00; C23C016-34; C23C016-40; C23C016-448  
 CC 47-7 (Apparatus and Plant Equipment)  
 Section cross-reference(s): 57, 75, 76  
 ST metalorg **CVD** barium strontium titanate dielec; electrode  
 dielec oxide metalorg **CVD**; metal nitride film **CVD**  
 ; vapor transport carrier gas dielec film **CVD**  
 IT **Vapor deposition** process  
 (chem.; film formation by **CVD** for dielec.  
 devices)  
 IT Electric insulators  
 Electrodes  
 (film formation by **CVD** for dielec. devices)  
 IT 1304-28-5P, Barium oxide, uses 1305-78-8P, Calcium oxide, uses  
 1314-11-0P, Strontium oxide, uses 1314-23-4P, Zirconia, uses  
 1314-61-0P, Tantalum oxide (Ta205) 1317-36-8P, Lead oxide (PbO),  
 uses 7440-50-8P, Copper, uses 12033-62-4P, Tantalum nitride  
 (TaN) 12058-38-7P, Tungsten nitride (WN) 12673-59-5P, Niobium  
 Strontium oxide 25583-20-4P, Titanium nitride (TiN) 39427-01-5P,  
 Aluminum copper oxide 106603-81-0P, Strontium tantalum oxide  
 (film formation by **CVD** for dielec. devices)  
 IT 64-17-5, Ethanol, processes 75-04-7, Monoethyl amine, processes  
 75-64-9, tert-Butylamine, processes 109-89-7, processes 112-24-3  
 112-57-2, Tetraethylene pentamine 124-40-3, Dimethylamine,  
 processes 598-56-1 754-05-2, Trimethylvinyl silane 1118-71-4  
 3236-82-6 6074-84-6 7784-21-6, Aluminum hydride 14781-45-4,  
 Bis(hexafluoroacetylacetone copper) 16761-83-4 17594-47-7,  
 Bis(Dipivaloylmethanato barium) 36830-74-7,  
 Bis(Dipivaloylmethanato strontium) 55161-66-5 59196-92-8  
 61156-35-2 **67313-80-8** 118448-18-3,  
 Bis(Dipivaloylmethanato calcium) 150178-00-0,  
 Bis(Dipivaloylmethanato lead) **169896-41-7** 184675-46-5  
 245655-35-0 261929-98-0  
 (film formation by **CVD** for dielec. devices)  
 IT 7440-25-7P, Tantalum, uses 7440-32-6P, Titanium, uses  
 7440-33-7P, Tungsten, uses  
 (wiring; film formation by **CVD** for dielec. devices)  
 L23 ANSWER 10 OF 19 HCA COPYRIGHT 2001 ACS  
 132:230668 Method for forming a three-component nitride film containing  
 metal and silicon for semiconductor device fabrication. Yi,  
Kyoung-soo; Koh, Won-yong; Kang, Sang-won (Genitech Co., Ltd., S.  
 Korea). PCT Int. Appl. WO 2000016377 A2 20000323, 13 pp.  
 DESIGNATED STATES: W: JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI,  
 FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2.  
 APPLICATION: WO 1999-KR534 19990910. PRIORITY: KR 1998-37257  
 19980910; KR 1998-48993 19981116.  
 AB The method of the present invention comprises the steps of: prepg.  
 sep. reactive gases each including at least one selected from the  
 group consisting of a gaseous metal compd., a gaseous Si compd. and  
 an NH<sub>3</sub> gas under conditions such that the gaseous metal compd. and  
 the NH<sub>3</sub> gas does not form a mixt.;. Detg. a sequential gas supply

cycle of the reactive gases so that supplies of the gaseous metal compd., the gaseous Si compd. and the NH<sub>3</sub> gas are each included at least once within one gas supply cycle; and applying the reactive gases to the substrate by repeating the gas supply cycle at least once. According to the present invention, a three-component nitride film can be formed with a uniform thickness despite unevenness of a semiconductor substrate surface.

IT 169896-41-7, Tris(diethylamido)(tert-butylimido)tantalum  
(method for forming three-component nitride film contg. metal and silicon for semiconductor device fabrication)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM H01L

CC 76-3 (Electric Phenomena)

ST Section cross-reference(s): 75

ST OMCVD metal nitride silicide film

IT 3275-24-9, Tetrakis(dimethylamido)titanium 4419-47-0,  
Tetrakis(diethylamido)titanium 7664-41-7, Ammonia, reactions  
7803-62-5, Silane, reactions 169896-41-7,  
Tris(diethylamido)(tert-butylimido)tantalum  
(method for forming three-component nitride film contg. metal and silicon for semiconductor device fabrication)

L23 ANSWER 11 OF 19 HCA COPYRIGHT 2001 ACS

132:29908 Niobium and tantalum derivatives with bidentate nitrogen ligands as potential precursors to nitrides. Hubert-Pfalzgraf, L. G.; Decams, J.-M.; Daniele, S. (Universite Claude Bernard - Lyon I, UMR-CNRS, Villeurbanne, 69622, Fr.). J. Phys. IV, 9(Pr8), Proceedings of the Twelfth European Conference on Chemical Vapour Deposition, 1999, Vol. 2), 953-958 (English) 1999. CODEN: JPICEI. ISSN: 1155-4339. Publisher: EDP Sciences.

AB Early transition metal derivs. with N-donors have attracted interest as precursors of nitrides, the latter being used as diffusion barriers for the ULSI technol. Potential precursors to niobium and tantalum nitrides were synthesized in good yields and characterized. They are based on bidentate nitrogen donors amidinates, benzamidinates and diamido ligands. These were reacted with niobium or tantalum penta- and tetra-chlorides and TaCl<sub>3</sub>(NET<sub>2</sub>)<sub>2</sub>. Disubstituted niobium(IV) and tantalum(V) species such as NbCl<sub>2</sub>[RNCR'NR<sub>2</sub>]<sub>2</sub> [R = Cy, N(SiMe<sub>3</sub>)<sub>2</sub>; R' = SiMe<sub>3</sub>, R' = p-tolyl] were obtained and structurally characterized. The more rigid o-dimethylphenylene diamido ligand leads to the volatile, air stable

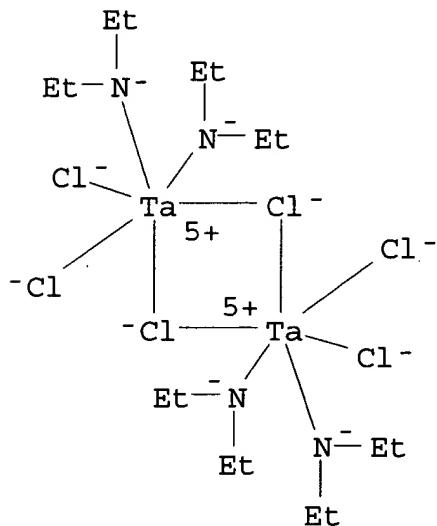
disubstituted Nb(V) species  $\text{NbCl}\{\text{N}_2(\text{SiMe}_3)_2\text{C}_6\text{H}_2\text{Me}_2\}_2$ . However,  $\pi$ -stacking as shown by x-ray studies are responsible of quite low sublimation rates. Thus, volatility could be reached for some species, their properties, high solv. due to the trimethylsilyl ligands, their stability in soln. is more suited for applications in wet MOCVD than conventional one.

IT 122539-86-0

(for prepn. of tantalum benzamidinato and guanidinato diethylamido chloro complexes as potential nitride precursors)

RN 122539-86-0 HCA

CN Tantalum, di-.mu.-chlorotetrachlorotetrakis(N-ethylethanaminato)di-, stereoisomer (9CI) (CA INDEX NAME)

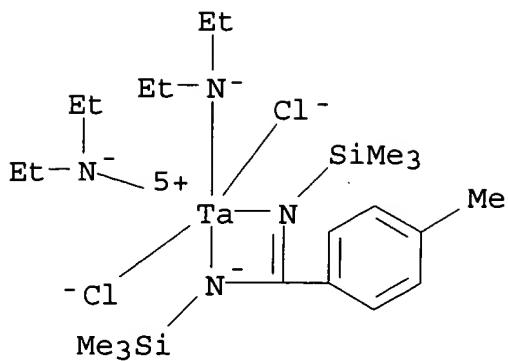


IT 251932-31-7P 251932-32-8P

(prepn. as potential nitride precursor)

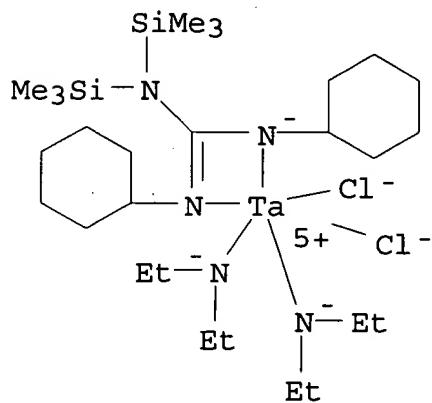
RN 251932-31-7 HCA

CN Tantalum, dichlorobis(N-ethylethanaminato) [4-methyl-N,N'-bis(trimethylsilyl)benzenecarboximidamido-.kappa.N,.kappa.N']- (9CI) (CA INDEX NAME)



RN 251932-32-8 HCA

CN Tantalum, dichloro[N',N''-dicyclohexyl-N,N-bis(trimethylsilyl)guanidinato-.kappa.N',.kappa.N'']bis(N-ethylethanaminato)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT 122539-86-0

(for prepn. of tantalum benzamidinato and guanidinato diethylamido chloro complexes as potential nitride precursors)

IT 251932-29-3P 251932-30-6P 251932-31-7P

251932-32-8P

(prepn. as potential nitride precursor)

L23 ANSWER 12 OF 19 HCA COPYRIGHT 2001 ACS

130:183429 Composite material and its manufacture. Breme, Frank,  
Guther, Volker; Van Osten, Karl-Uwe (GfE Metalle und Materialien  
G.m.b.H., Germany). Eur. Pat. Appl. EP 897997 A1 19990224, 15 pp.  
DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI,  
LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (German). CODEN:  
EPXXDW. APPLICATION: EP 1998-115821 19980821. PRIORITY: DE  
1997-19736449 19970821.

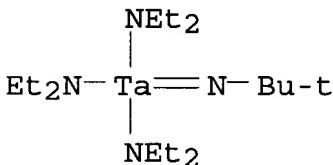
AB The composites comprise a plastic substrate and a deposited continuous layer (thickness <2 .mu.m) of a ductile metal-contg. compd.  $MaObCxNyBz$  ( $M = Ti, Ta, Nb, Zr, Hf; a = 0.025-0.9; b = 0.025-0.7; x = 0.2-0.9; y, z = 0-0.7; a + b + x + y + z = 1$ ) such that the  $M$  concn. (a) increases continuously from the substrate interface (where  $a$  is .apprxeq.0) to the surface of the deposited layer, and are prep'd. by activating the plastic surface, vapor-depositing an appropriate metal compd. at  $\approx 100$  degree., and treating with a plasma at <50 millibars. The products find use in medical technol. as prostheses, etc. Thus, poly(ethylene terephthalate) was surface-treated with a 50-W inductive plasma (13.56 MHz) for 3 min at .apprx.1 millibar, heated to .apprx.100. degree., then treated with  $Ti(NMe_2)_4$  vapors in a H carrier gas stream at 5. degree., and exposed to a low-pressure plasma. The coating adhered to the substrate with peel strength >6 N/mm<sup>2</sup> and showed cond. 2.1 (.OMEGA.-cm)-1 initially, which decreased to 0.18 (.OMEGA.-cm)-1 after 3 days exposure to air.

IT 169896-41-7

(composite material by CVD of)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM C23C016-30

ICS C23C016-18; C23C016-02

CC 38-2 (Plastics Fabrication and Uses)

Section cross-reference(s): 42, 57, 63

ST ceramic thermoplastic composite prosthesis; **chem**

**vapor deposition** plasma assisted

IT Prosthetic composites

(ceramic-plastic; manuf. of composite materials by CVD)

IT **Chemical vapor deposition**

(in manuf. of composite materials)

IT Plasma

(low-pressure; in manuf. of composite materials by CVD)

IT Fluoropolymers, uses

Polyamides, uses

Polyesters, uses

Polyurethanes, uses

(substrate; composite material by CVD on)

IT 1333-74-0, Hydrogen, uses

(carrier gas; in manuf. of composite materials by CVD)

IT 3275-24-9, Tetrakis(dimethylamino)titanium 19824-58-9, Pentakis(dimethylamino)niobium 19824-59-0,

Pentakis(dimethylamino)tantalum 25169-05-5,  
 Pentakis(diethylamino)niobium 55161-66-5,  
 Pentakis(diethylamido)tantalum 169896-41-7 210363-27-2  
 (composite material by CVD of)

IT 9002-84-0, PTFE 9003-07-0, Polypropylene 25038-59-9,  
 Poly(ethylene terephthalate), uses  
 (substrate; composite material by CVD on)

L23 ANSWER 13 OF 19 HCA COPYRIGHT 2001 ACS

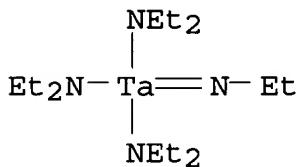
129:297190 CVD of nitride layers in semiconductor device fabrication. Jain, Ajay; Weitzman, Elizabeth (Motorola, Inc., USA). Eur. Pat. Appl. EP 869544 A2 19981007, 8 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 1998-104865 19980318. PRIORITY: US 1997-829752 19970331.

AB Refractory metal nitride and refractory metal Si nitride layers can be formed by metalorg. chem. vapor deposition. More specifically, TaN can be formed by CVD using ethyltris(diethylamido)tantalum (ETDET) and NH<sub>3</sub>. By the inclusion of SiH<sub>4</sub>, a TaSiN layer can also be formed. Both of these layers can be formed at wafer temps.  $\sim 400$ .degree. with relatively small amts. of C within the film. The invention can be used to form TaN or TaSiN that is relatively conformal and has reasonably good diffusion barrier properties.

IT 67313-80-8  
 (ETDET; in CVD of nitride diffusion barrier layers in semiconductor device fabrication)

RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)  
 (CA INDEX NAME)



IC ICM H01L021-285  
 CC 76-3 (Electric Phenomena)  
 Section cross-reference(s): 75

ST MOCVD diffusion barrier semiconductor device; tantalum nitride MOCVD semiconductor device; silicon tantalum nitride MOCVD semiconductor device

IT Diffusion barrier  
 (CVD of nitride diffusion barrier layers in semiconductor device fabrication)

IT Semiconductor device fabrication  
 (CVD of nitride layers in)

IT Refractory metal compounds  
 (nitrides; CVD of nitride layers in semiconductor

device fabrication)

IT Metalorganic **chemical vapor deposition**  
(of nitride layers in semiconductor device fabrication)

IT 12033-62-4, Tantalum nitride 99039-55-1, Tantalum nitride silicide  
(CVD of nitride diffusion barrier layers in  
semiconductor device fabrication)

IT **67313-80-8**  
(ETDET; in **CVD** of nitride diffusion barrier layers in  
semiconductor device fabrication)

L23 ANSWER 14 OF 19 HCA COPYRIGHT 2001 ACS

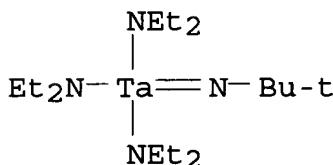
127:271322 Fabricating a tantalum nitride diffusion barrier for copper  
metalization. Sun, Shi-chung; Chiu, Hien-tien; Tsai, Ming-hsing  
(United Microelectronics Corp., Taiwan). U.S. US 5668054 A  
19970916, 10 pp. (English). CODEN: USXXAM. APPLICATION: US  
1996-584749 19960111.

AB A process for fabricating a TaN diffusion barrier for the advanced  
Cu metalization of semiconductor devices is disclosed. The process  
comprises prep. a semiconductor device fabricated over the surface  
of a Si substrate having a component with a fabricated contact  
opening. Before the formation of the Cu contact by deposition, the  
process performs a TaN low-pressure **CVD** procedure that  
deposits a TaN film over the substrate. After the Cu deposition, a  
photoresist layer is subsequently fabricated for patterning the  
deposited Cu contact and TaN layers, whereby the deposited film of  
TaN is patterned to form the metalization diffusion barrier for the  
semiconductor device. The TaN low-pressure **CVD** procedure  
includes depositing a layer of TaN using the metalorg. precursor  
tert-butylimido-tris(diethylamido)tantalum (TBTDET) in a cold-wall  
low-pressure reactor with a base pressure of .apprx.10-5 torr. The  
source of the metalorg. precursor is vaporized at  
.apprx.40-50.degree.. The typical deposition pressure is .apprx.20  
mtoorr. A TaN layer of low C content and low resistivity may thus be  
formed in the disclosed **CVD** procedure having effective  
capability against Cu diffusion.

IT **169896-41-7**, Tertbutylimidotris(Diethylamido)tantalum  
(fabricating a tantalum nitride diffusion barrier for copper  
metalization by **CVD** from)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethyllethanaminato)[2-methyl-2-propanaminato(2-)]-,  
(T-4)- (9CI) (CA INDEX NAME)



IC ICM H01L021-28  
NCL 438653000

CC 76-3 (Electric Phenomena)  
 IT **Chemical vapor deposition**  
     (of tantalum nitride diffusion barrier for copper metalization in  
     a semiconductor device)  
 IT **169896-41-7, Tertbutylimidotris(Diethylamido)tantalum**  
     (fabricating a tantalum nitride diffusion barrier for copper  
     metalization by CVD from)

L23 ANSWER 15 OF 19 HCA COPYRIGHT 2001 ACS

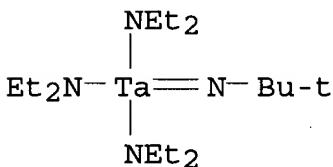
126:285955 Properties of metalorganic **chemical vapor**  
**deposited** tantalum nitride thin films. Sun, S. C.; Tsai, M.  
 H.; Tsai, C. E.; Chiu, H. T. (National Nano Device Laboratory,  
 Institute of Electronics, National Chiao Tung University, Taipei,  
 Peop. Rep. China). Proc. - Int. Conf. Solid-State Integr. Circuit  
 Technol., 4th, 547-549. Editor(s): Baldwin, Gary L. Institute of  
 Electrical and Electronics Engineers: New York, N. Y. (English)  
 1995. CODEN: 64CRAT.

AB Low-resistivity Ta nitride (TaN) films were successfully realized by  
 low-pressure metalorg. CVD using a new precursor TBTDET  
 (tertbutylimido-tris-diethylamino Ta). Data from TEM and XRD anal.  
 indicated that 600.degree. as-deposited films exhibit the polycryst.  
 structure with <200> preferred orientation. CVD TaN films  
 were studied as diffusion barriers for Cu and Al interconnections.

IT **169896-41-7**  
     (starting material; properties of MOCVD tantalum  
     nitride thin films)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-,  
 (T-4)- (9CI) (CA INDEX NAME)



CC 76-2 (Electric Phenomena)  
 Section cross-reference(s): 75  
 ST **MOCVD tantalum nitride film; resistance tantalum nitride**  
     **film; diffusion barrier tantalum nitride film**  
 IT Diffusion barrier  
     Electric resistance  
     Polycrystalline films  
         (properties of MOCVD tantalum nitride thin films)  
 IT Metalorganic **chemical vapor deposition**  
         (properties of MOCVD tantalum nitride thin films)  
 IT 7440-44-0, Carbon, occurrence 7782-44-7, Oxygen, occurrence  
         (properties of MOCVD tantalum nitride thin films)  
 IT 12033-62-4P, Tantalum nitride (TaN)  
         (properties of MOCVD tantalum nitride thin films)

IT 169896-41-7

(starting material; properties of MOCVD tantalum nitride thin films)

L23 ANSWER 16 OF 19 HCA COPYRIGHT 2001 ACS

126:164537 Process for the preparation of metal nitride coatings from single source precursors. Winter, Charles H.; Lewkebandara, T. Suren; Jayaratne, Kumudini C. (Wayne State University, USA). U.S. US 5591483 A 19970107, 8 pp. (English). CODEN: USXXAM.

APPLICATION: US 1994-298764 19940831.

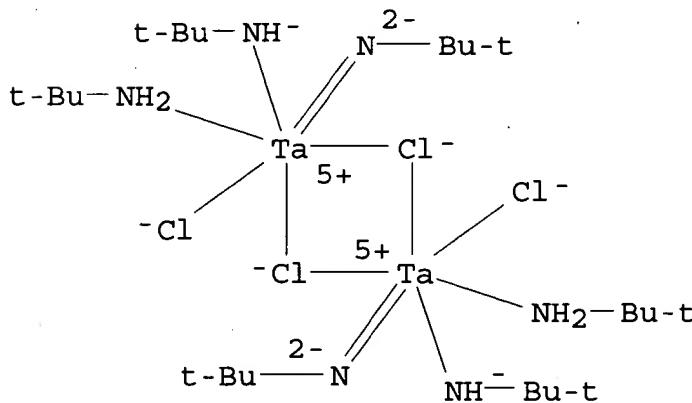
AB Metal nitride coatings are deposited effectively by the decompn. of single source metal imido-amidoamine precursors prep'd. by the reaction of a pentavalent metal halide with a primary amine or hydrazine. Preferably the compds. derived from a pentavalent metal M have the formula  $[MCl_2(NR)(NHR)(NH_2R)]_n$ , where R is alkyl, cycloalkyl, aryl, cycloalkenyl, or NR<sub>1</sub>R<sub>2</sub>, where R<sub>1</sub> and R<sub>2</sub> are independently alkyl, cycloalkyl, alkenyl, cycloalkenyl, aryl, or hydrogen, and where n is a whole no. from 1 to 3, while the compds. derived from a tetravalent metal M' have the formula  $[M'Cl_2(NNR_1R_2)(NH_2NR_1R_2)]_n$ , where R<sub>1</sub> and R<sub>2</sub> have the same meanings as above, or together with the nitrogen to which they are bonded from a cyclic imine, and where n is a whole no. from 1 to 3, preferably 2. With hydrazine-derived precursors, TaN coatings may be deposited as low as 400.degree. or lower.

IT 90836-77-4P 158990-06-8P

(prepn. as single source precursor for tantalum nitride film deposition)

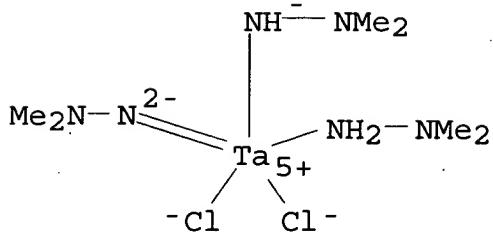
RN 90836-77-4 HCA

CN Tantalum, di-.mu.-chlorodichlorobis(2-methyl-2-propanaminato)bis[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)



RN 158990-06-8 HCA

CN Tantalum, dichloro(1,1-dimethylhydrazinato-N2) [1,1-dimethylhydrazinato(2-)-N2] (1,1-dimethylhydrazine-N2)- (9CI) (CA INDEX NAME)



IC ICM C23C016-00  
 NCL 427248100  
 CC 75-1 (Crystallography and Liquid Crystals)  
 ST nitride metal film CVD single precursor; tantalum nitride  
 film CVD single precursor  
 IT Nitrides  
 (CVD of metal nitrides using single source precursor)  
 IT Chemical vapor deposition  
 (of metal nitrides using single source precursor)  
 IT 90836-77-4P 158990-06-8P  
 (prepn. as single source precursor for tantalum nitride film  
 deposition)

L23 ANSWER 17 OF 19 HCA COPYRIGHT 2001 ACS

125:211211 Imido Complexes Derived from the Reactions of Niobium and  
 Tantalum Pentachlorides with Primary Amines: Relevance to the  
 Chemical Vapor Deposition of Metal  
 Nitride Films. Jayaratne, Kumudini C.; Yap, Glenn P. A.; Haggerty,  
 Brian S.; Rheingold, Arnold L.; Winter, Charles H. (Department of  
 Chemistry, Wayne State University, Detroit, MI, 48202, USA). Inorg.  
 Chem., 35(17), 4910-4920 (English) 1996. CODEN: INOCAJ. ISSN:  
 0020-1669.

AB Reactions of NbCl<sub>5</sub> and TaCl<sub>5</sub> with tert-butylamine (.gtoreq.6 equiv)  
 in benzene afford the dimeric imido complexes  
 $[\text{NbCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$  (90%) and  
 $[\text{TaCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$  (79%). The Nb complex exists as two  
 isomers in soln., while the Ta complex is composed of three major  
 isomers and at least two minor isomers. Analogous treatments with  
 isopropylamine (.gtoreq.7 equiv) give the monomeric complexes  
 $\text{NbCl}_2(\text{NiPr})(\text{NHiPr})(\text{NH}_2\text{iPr})_2$  (84%) and  $\text{TaCl}_2(\text{NiPr})(\text{NHiPr})(\text{NH}_2\text{iPr})_2$   
 (84%). The monomeric complexes are unaffected by treatment with  
 excess isopropylamine, while the dimeric complexes are cleaved to  
 the monomers  $\text{MC}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})_2$  upon addn. of excess  
 tert-butylamine in CHCl<sub>3</sub> soln. Treatment of NbCl<sub>5</sub> and TaCl<sub>5</sub> with  
 2,6-diisopropylaniline affords insol. ppts. of  $[\text{NH}_3(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3)]_2[\text{NbCl}_5(\text{N}(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3))]$  (100%) and  
 $[\text{NH}_3(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3)]_2[\text{TaCl}_5(\text{N}(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3))]$  (100%), which  
 react with 4-tert-butylpyridine to afford the sol. complexes  
 $[4-t-\text{C}_4\text{H}_9\text{C}_5\text{H}_4\text{NH}]_2[\text{NbCl}_5(\text{N}(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3))]$  (45%) and  
 $[4-t-\text{C}_4\text{H}_9\text{C}_5\text{H}_4\text{NH}]_2[\text{TaCl}_5(\text{N}(2,6-(\text{CHMe}_2)_2\text{C}_6\text{H}_3))]$  (44%). Sublimation of

$[\text{NbCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$ ,  $\text{MCl}_2(\text{NiPr})(\text{NHtBu})(\text{NH}_2\text{iPr})_2$ , and  $[\text{NH}_3(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3)]_2[\text{MCl}_5(\text{N}(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))]$  leads to disproportionation to give  $[\text{MCl}_3(\text{NR})(\text{NH}_2\text{R})]_2$  as sublimates (32-49%), leaving complexes of the proposed formulation  $\text{MC}_1(\text{NR})_2$  as nonvolatile residues. By contrast,  $[\text{TaCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$  sublimes without chem. reaction. Anal. of the org. products obtained from thermal decompn. of  $[\text{NbCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$  showed isobutylene and tert-butylamine in a 2.2:1 ratio. Mass spectra of  $[\text{NbCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$ ,  $[\text{TaCl}_2(\text{NtBu})(\text{NHtBu})(\text{NH}_2\text{tBu})]_2$ , and  $[\text{NbCl}_3(\text{NiPr})(\text{NH}_2\text{iPr})]_2$  showed dimeric imido complexes, monomeric imido complexes, and nitrido complexes, implying that such species are important gas phase species in CVD processes using these mol. precursors.  $[\text{4-T-C}_4\text{H}_9\text{C}_5\text{H}_4\text{NH}]_2[\text{NbCl}_5(\text{N}(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))]$  crystallizes in the space group  $\text{P}2_1/\text{c}$  with a  $12.448(3)$ ,  $b 10.363(3)$ ,  $c 28.228(3)$  .ANG.,  $\beta 94.92(1)$ .degree., and  $Z = 4$ .  $[\text{NbCl}_3(\text{NiPr})(\text{NH}_2\text{iPr})]_2$  crystallizes in the space group  $\text{P}2_1/\text{c}$  with a  $9.586(4)$ ,  $b 12.385(4)$ ,  $c 11.695(4)$  .ANG.,  $\beta 112.89(2)$ .degree., and  $Z = 2$ .  $[\text{NbCl}_3(\text{N}(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))(\text{NH}_2(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))]_2$  crystallizes in the space group  $\text{P}2_1/\text{n}$  with a  $10.285(3)$ ,  $b 11.208(3)$ ,  $c 23.867(6)$  .ANG.,  $\beta 97.53$ .degree., and  $Z = 2$ .  $[\text{TaCl}_3(\text{N}(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))(\text{NH}_2(2,6-(\text{CHMe}_2)2\text{C}_6\text{H}_3))]_2$  crystallizes in the space group  $\text{P}2_1/\text{n}$  with a  $10.273(1)$ ,  $b 11.241(2)$ ,  $c 23.929(7)$  .ANG.,  $\beta 97.69(2)$ .degree., and  $Z = 2$ . These findings are discussed in the context of Nb and Ta nitride film depositions from mol. precursors.

IT

90836-77-4P 180966-34-1P

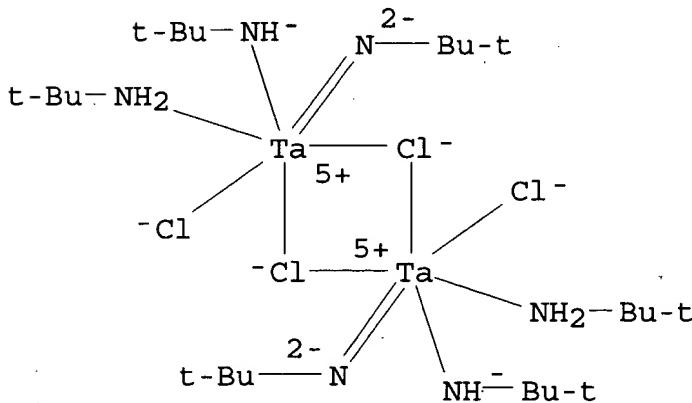
(prepn. as CVD precursor and decompn. during attempted sublimation)

RN

90836-77-4 HCA

CN

Tantalum, di-.mu.-chlorodichlorobis(2-methyl-2-propanaminato)bis[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)

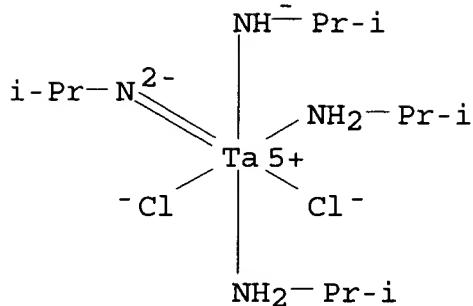


RN

180966-34-1 HCA

CN

Tantalum, dichloro(2-propanaminato)[2-propanaminato(2-)]bis(2-propanamine)- (9CI) (CA INDEX NAME)

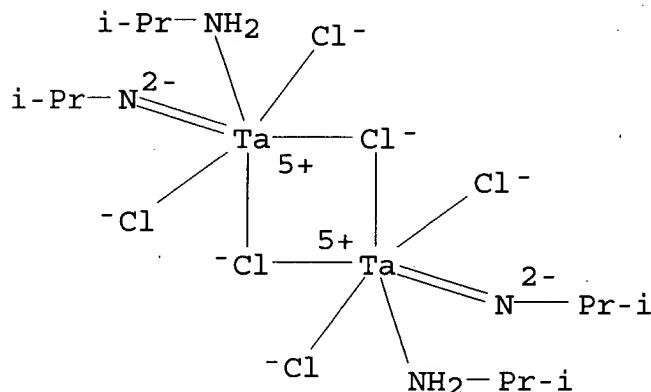


IT 180966-42-1P

(prepn. by decompn. of CVD precursor during attempted sublimation)

RN 180966-42-1 HCA

CN Tantalum, di-.mu.-chlorotetrachlorobis[2-propanaminato(2-)]bis(2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)

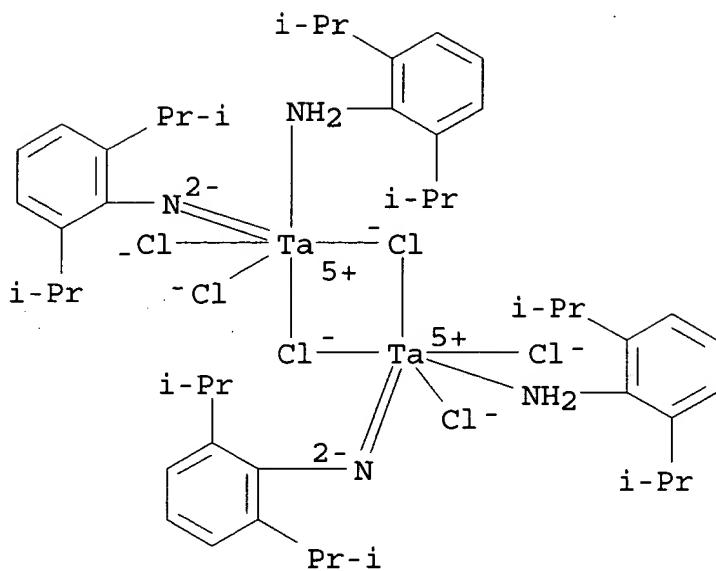


IT 180966-44-3P

(prepn. by decompn. of CVD precursor during attempted sublimation and crystal structure of)

RN 180966-44-3 HCA

CN Tantalum, bis[2,6-bis(1-methylethyl)benzenaminato(2-)]bis[2,6-bis(1-methylethyl)benzenamine]di-.mu.-chlorotetrachlorodi-, stereoisomer (9CI) (CA INDEX NAME)

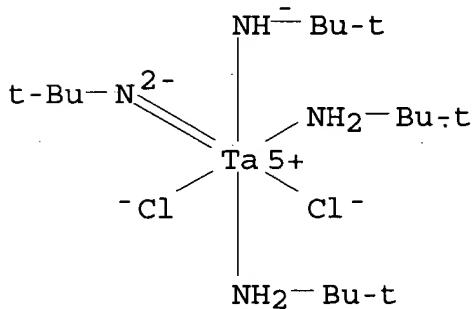


IT 180966-48-7P

(prepn. of)

RN 180966-48-7 HCA

CN Tantalum, dichloro(2-methyl-2-propanaminato)[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine)- (9CI) (CA INDEX NAME)



CC 78-9 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

ST crystal structure niobium tantalum imido chloro; structure niobium tantalum imido CVD precursor; niobium imido chloro prep CVD precursor; tantalum imido chloro prep CVD precursor; imido niobium tantalum prep CVD precursor; thermal reaction niobium tantalum imido CVD; sublimation niobium tantalum imido CVD mechanism; decompn niobium tantalum imido thermal CVD; nitride film niobium tantalum precursor CVD

IT Sublimation

(decompn. during attempted sublimation of niobium and tantalum mixed imido amine **CVD** precursors)

IT Disproportionation  
Thermal decomposition  
(of niobium and tantalum mixed imido amine **CVD** precursors during attempted sublimation)

IT Imides  
(complexes, niobium and tantalum chloro amine and amide; prepn. as **CVD** precursors and thermal decompn. during attempted sublimation)

IT Reaction mechanism  
(gas-phase, decompn. of niobium and tantalum mixed imido amine **CVD** precursors during attempted sublimation)

IT 75-31-0, Isopropylamine, reactions 75-64-9, tert-Butylamine, reactions 24544-04-5, 2,6-Diisopropylaniline  
(for prepn. of niobium and tantalum imido amido amine chloro complexes as **CVD** precursors)

IT 10026-12-7, Niobium chloride (NbCl<sub>5</sub>)  
(for prepn. of niobium imido amine chloro complexes as **CVD** precursors)

IT 7721-01-9, Tantalum chloride (TaCl<sub>5</sub>)  
(for prepn. of tantalum imido amido amine chloro complexes as **CVD** precursors)

IT 115-11-7, Isobutylene, formation (nonpreparative) 180966-46-5  
(formation by thermal decompn. of niobium imido amido amine chloro **CVD** precursor)

IT 180966-39-6P  
(prepn. as **CVD** precursor)

IT 180966-40-9P  
(prepn. as **CVD** precursor and crystal structure of)

IT 90836-77-4P 90836-78-5P 180966-33-0P  
180966-34-1P 180966-36-3P 180966-38-5P  
(prepn. as **CVD** precursor and decompn. during attempted sublimation)

IT 180966-42-1P 181141-01-5P  
(prepn. by decompn. of **CVD** precursor during attempted sublimation)

IT 180966-41-0P 180966-43-2P 180966-44-3P  
(prepn. by decompn. of **CVD** precursor during attempted sublimation and crystal structure of)

IT 180966-47-6P 180966-48-7P  
(prepn. of)

L23 ANSWER 18 OF 19 HCA COPYRIGHT 2001 ACS

124:329193 Performance of **MOCVD** tantalum nitride diffusion barrier for copper metalization. Sun, S. C.; Tsai, M. H.; Tsai, C. E.; Chiu, H. T. (Department Electronics Engineering, National Chiao Tung University, Hsinchu, Taiwan). Symp. VLSI Technol., Dig. Tech. Pap., 15th, 29-30. Business Center for Academic Societies Japan: Tokyo, Japan. (English) 1995. CODEN: 62PWAR.

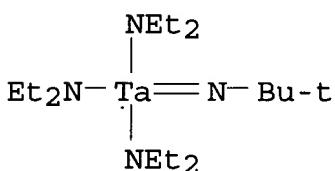
AB A low-resistivity and low C concn. **CVD** TaN film was realized by using a new precursor terbutylimido-tris-diethylamido Ta

(TBTDET). CVD TaN as a diffusion barrier for Cu has higher thermal stability up to 500.degree. than CVD TiN of 450.degree..

IT 169896-41-7, Tertbutylimido-tris-diethylamido Tantalum (performance of MOCVD tantalum nitride diffusion barrier for copper metalization)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



CC 76-2 (Electric Phenomena)

Section cross-reference(s): 75

ST MOCVD tantalum nitride diffusion barrier copper; metalization copper interconnection diode

IT Diodes

Vapor deposition processes

(performance of MOCVD tantalum nitride diffusion barrier for copper metalization)

IT Electric conductors

(interconnections, performance of MOCVD tantalum nitride diffusion barrier for copper metalization)

IT 169896-41-7, Tertbutylimido-tris-diethylamido Tantalum (performance of MOCVD tantalum nitride diffusion barrier for copper metalization)

IT 12033-62-4P, Tantalum nitride (TaN) (performance of MOCVD tantalum nitride diffusion barrier for copper metalization)

L23 ANSWER 19 OF 19 HCA COPYRIGHT 2001 ACS

123:302763 Metalorganic chemical vapor

deposition of tantalum nitride by

tertbutylimidotris(diethylamido)tantalum for advanced metalization.

Tsai, M. H.; Sun, S. C.; Chiu, H. T.; Tsai, C. E.; Chuang, S. H.

(Institute Electronics, National Chiao Tung University, Hsinchu, 30050, Taiwan). Appl. Phys. Lett., 67(8), 1128-30 (English) 1995.

CODEN: APPLAB. ISSN: 0003-6951.

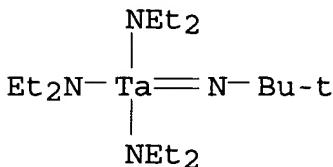
AB The authors deposited tantalum nitride (TaN) films by low-pressure metalorg. CVD (LP-MOCVD) using a new precursor

tertbutylimidotris(diethylamido)tantalum (TBTDET). Strong Ta-N double bond in the precursor preserved the TaN portion during the pyrolysis process. This method has yielded low-resistivity films.

It changed from 10 m.OMEGA. cm (deposited at 500.degree.) to 920 .mu..OMEGA. cm (obtained at 650.degree.). The carbon and oxygen concns. were low in the films deposited at 600.degree., as detd. by

XPS. TEM and x-ray diffraction anal. indicated that the as-deposited films exhibited polycryst. structures with the lattice consts. close to the bulk TaN value. The TaN barrier layer was successfully applied as a glue layer for CVD tungsten (W) metalization schemes.

IT 169896-41-7, Tertbutylimidotris(diethylamido)tantalum  
 (metalorg. chem. vapor deposition  
 of tantalum nitride by tertbutylimidotris(diethylamido)tantalum  
 for advanced metalization)  
 RN 169896-41-7 HCA  
 CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-,  
 (T-4) - (9CI) (CA INDEX NAME)



CC 76-2 (Electric Phenomena)  
 Section cross-reference(s): 75  
 ST metalorg chem vapor deposition  
 tantalum nitride; metalization tantalum nitride metalorg CVD  
 IT Electric contacts  
 Vapor deposition processes  
 (metalorg. chem. vapor deposition  
 of tantalum nitride by tertbutylimidotris(diethylamido)tantalum  
 for advanced metalization)  
 IT 12033-62-4P, Tantalum nitride  
 (metalorg. chem. vapor deposition  
 of tantalum nitride by tertbutylimidotris(diethylamido)tantalum  
 for advanced metalization)  
 IT 169896-41-7, Tertbutylimidotris(diethylamido)tantalum  
 (metalorg. chem. vapor deposition  
 of tantalum nitride by tertbutylimidotris(diethylamido)tantalum  
 for advanced metalization)

=> d his 124-

(FILE 'HCA' ENTERED AT 13:48:44 ON 20 JUN 2001)

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001

FILE 'HCA' ENTERED AT 14:13:02 ON 20 JUN 2001

FILE 'LREGISTRY' ENTERED AT 14:15:37 ON 20 JUN 2001

L24 STR

FILE 'REGISTRY' ENTERED AT 14:17:28 ON 20 JUN 2001

L25 0 S L24 SSS SAM SUB=L11  
L26 4 S L24 SSS FUL SUB=L11  
SAV L26 PAD859C/A

FILE 'HCA' ENTERED AT 14:18:55 ON 20 JUN 2001

L27 3 S L26  
L28 2 S L27 NOT (L17 OR L22)

=> d 126 que stat

L9 STR

Ta $\vee$ G1	NH $\sim$ G2	N $\sim$ G2	@14 Ak $\sim$ F	@17 Si $\sim$ C	Ak @20
2      3	@5    6	@9    10	15	18	
			F	C	
			28	26	
			G2	C	
			24	27	25

VAR G1=NH2/5/9

VAR G2=20/PH/14/17

## NODE ATTRIBUTES:

```

NSPEC      IS  RC      AT   2
NSPEC      IS  RC      AT  18
NSPEC      IS  RC      AT  25
NSPEC      IS  RC      AT  26
CONNECT    IS  E1  RC  AT  20
DEFAULT    MLEVEL IS  ATOM
GGCAT      IS  SAT  AT  20
DEFAULT    ECLEVEL IS  LIMITED
ECOUNT     IS  M1-X4  C  AT  20

```

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9

L24 STR

Lewis structure of  $\text{Ta}(\text{NH}_3)_5\text{Cl}_2$ . The central Ta atom is bonded to five NH<sub>3</sub> ligands and two Cl<sup>-</sup> ligands. The NH<sub>3</sub> ligands are arranged in a distorted octahedral geometry around the Ta atom.

## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 6

## STEREO ATTRIBUTES: NONE

L26 4 SEA FILE=REGISTRY SUB=L11 SSS FUL L24

100.0% PROCESSED 85 ITERATIONS

SEARCH TIME: 00.00.01

4 ANSWERS

=&gt; d 128 1-2 ibib abs hitstr hitind

L28 ANSWER 1 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 83:70718 HCA

TITLE: Cyanate compounds and their reactivity. XXI.  
Reactivity of niobium(V) and tantalum(V)  
thiocyanates to nitrogen donators

AUTHOR(S): Boehland, H.; Harke, E.

CORPORATE SOURCE: Sekt. Chem. Biol., Paedagog. Hochsch. "Theodor  
Neubauer", Erfurt-Muehlhausen, E. Ger.SOURCE: Z. Anorg. Allg. Chem. (1975), 413(2), 102-8  
CODEN: ZAACAB

DOCUMENT TYPE: Journal

LANGUAGE: German

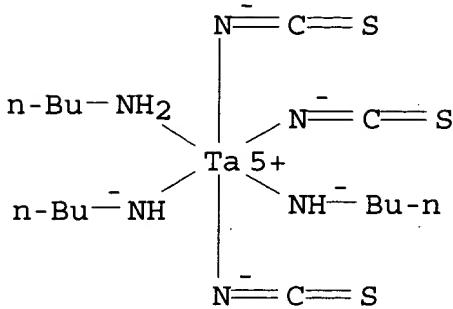
AB The preps. of  $[MeC(NH_2)_2]MX_6 \cdot 2MeCN$  (M = Ta, Nb; X = Cl, SCN),  
 $[M(NCS)(NC(NH_2)Me)_4(MeC(NH)NH_2)]_n$ ,  $[M(NCS)(NH_2)_2NH]_x$ ,  
 $[MeC(NH_2)_2][M(NCS)_4(NC(NH_2)Me)_2]$ ,  $[M(NCS)_3(NC(NHBu)Me)_2(MeC(NH)NHBu)]$ ,  
and  $[M(NCS)_3(NHBu)_2(BuNH_2)]$  are reported. The complexes are  
characterized by elemental anal., derivatog. measurements, and ir or  
visible absorption spectra.

IT 56142-56-4P

(prepn. of)

RN 56142-56-4 HCA

CN Tantalum, bis(1-butanaminato)(1-butanamine)tris(thiocyanato-N)-  
(9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)  
IT 56113-54-3P 56113-56-5P 56113-72-5P 56113-74-7P 56113-75-8P  
56113-76-9P 56113-78-1P 56113-79-2P **56142-56-4P**  
56142-57-5P 56214-94-9P 56214-95-0P 56227-53-3P 58004-49-2P  
(prepn. of)

L28 ANSWER 2 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 70:25323 HCA

TITLE: Reactions between acetonitrile and dialkylamido-compounds of titanium, zirconium, and tantalum

**AUTHOR(S):** Bradley, Donald C.; Ganorkar, M. C.

CORPORATE SOURCE: Queen Mary Coll., London, Engl.

SOURCE: Chem. Ind. (London) (1968), (44), 1521-2

CODEN: CHINAG

DOCUMENT TYPE: Journal

LANGUAGE : English

AB M(NMe<sub>2</sub>)<sub>x</sub>, where M = Ta, Zr, and Ti, were treated with y moles of MeCN to give M[N:C(Me)NMe<sub>2</sub>]<sub>y</sub>(NMe<sub>2</sub>)<sub>x-y</sub>. The ir spectra of these compds. showed a strong band in the 1577-87 cm.<sup>-1</sup> region which was attributed to the NCN group of the dimethylaminoacetaldimino ligand formed by insertion of MeCN in the M-NMe<sub>2</sub> bond. The compds. prep'd. and their characteristic ir bands were Ti[N:C(Me)NMe<sub>2</sub>](NMe<sub>2</sub>)<sub>3</sub> (I) 1580, Ti[N:C(Me)NMe<sub>2</sub>]<sub>2</sub>(NMe<sub>2</sub>)<sub>2</sub> (II) 1577, Zr[N:C(Me)-NMe<sub>2</sub>]<sub>4</sub> (III) 1587, Ta[N:C(Me)NMe<sub>2</sub>](NMe<sub>2</sub>)<sub>4</sub> (IV) 1585 cm.<sup>-1</sup> Hydrolysis of these compds. gave Me<sub>2</sub>NH and MeCN. Treatment of Ti(NEt<sub>2</sub>)<sub>4</sub> or Zr(NEt<sub>2</sub>)<sub>4</sub> with MeCN probably gave Et<sub>2</sub>NH and Ti(N:C:CH<sub>2</sub>)<sub>2</sub> or Zr(N:C:CH<sub>2</sub>)<sub>2</sub> although their ir spectra had the characteristic bands at 1560 and 1587 cm.<sup>-1</sup>, resp., assoc'd. with compds. I-IV.

IT 24980-83-4P

(prepn. of)

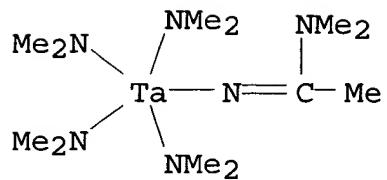
RN 24980-83-4 HCA

CN Tantalum, (N,N-dimethylacetamidinato)tetrakis(dimethylaminato)-, polymers (8CI) (CA INDEX NAME).

CM 1

CRN 45231-66-1

CMF C12 H33 N6 Ta



CC 78 (Inorganic Chemicals and Reactions)  
IT 21846-42-4P 21846-44-6P **24980-83-4P** 27081-65-8P  
27081-66-9P 27157-35-3P 27157-36-4P  
(prep. of)